

SUPPORTING INFORMATION FOR:

Potent combretastatin A-4 analogues containing quinoline: Design, Synthesis, antiproliferative, and anti-tubulin activity

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Figure S1; ¹H NMR for compound 19a

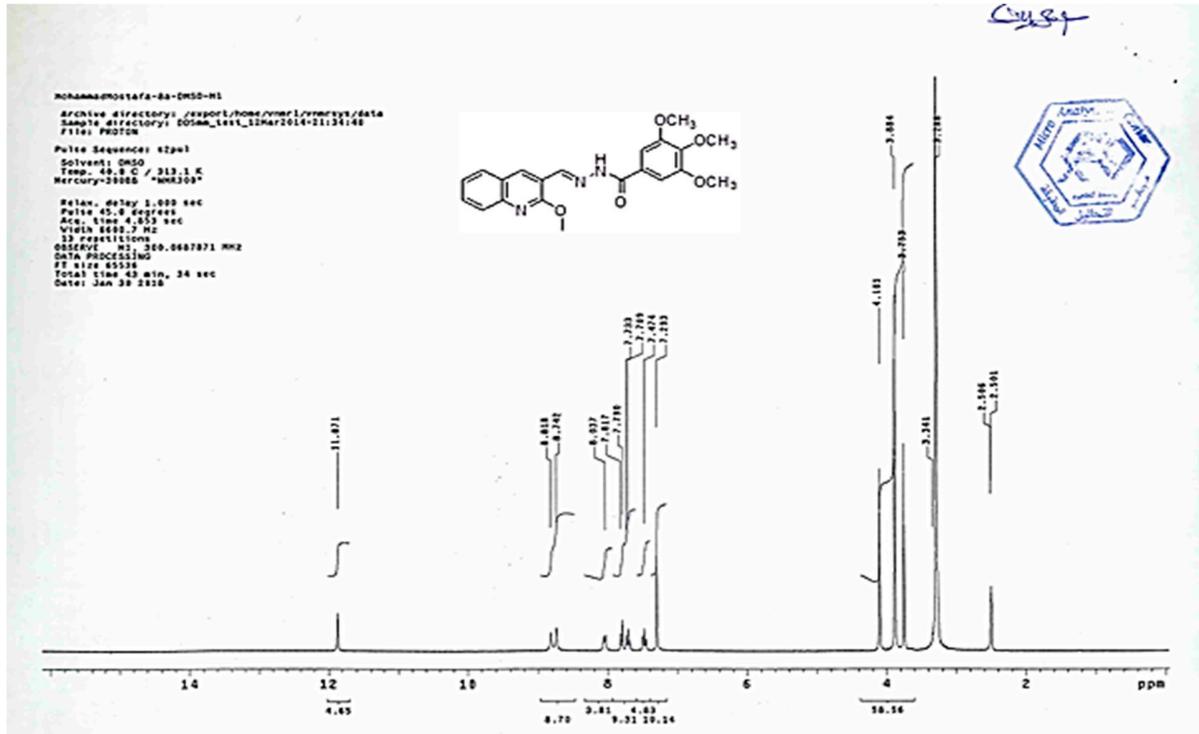


Figure S2; ¹³C NMR for compound 19a

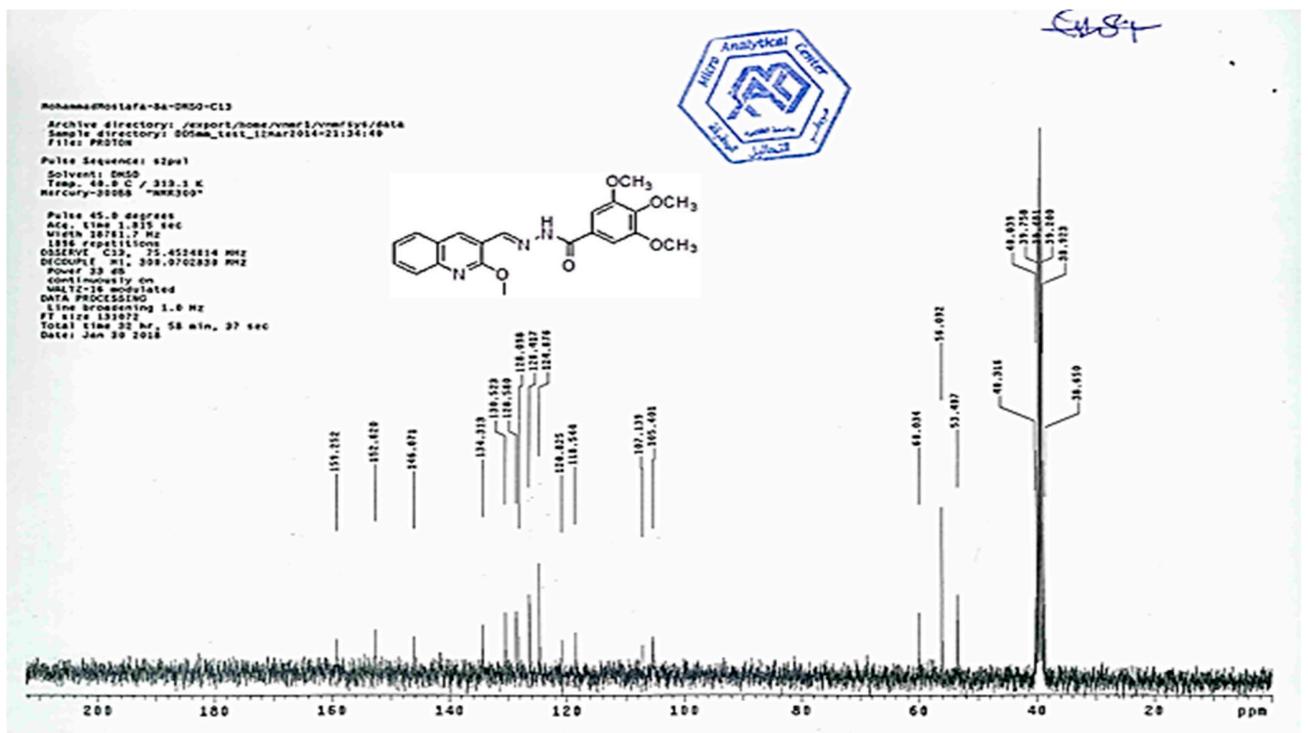


Figure S3; ¹H NMR for compound 19b

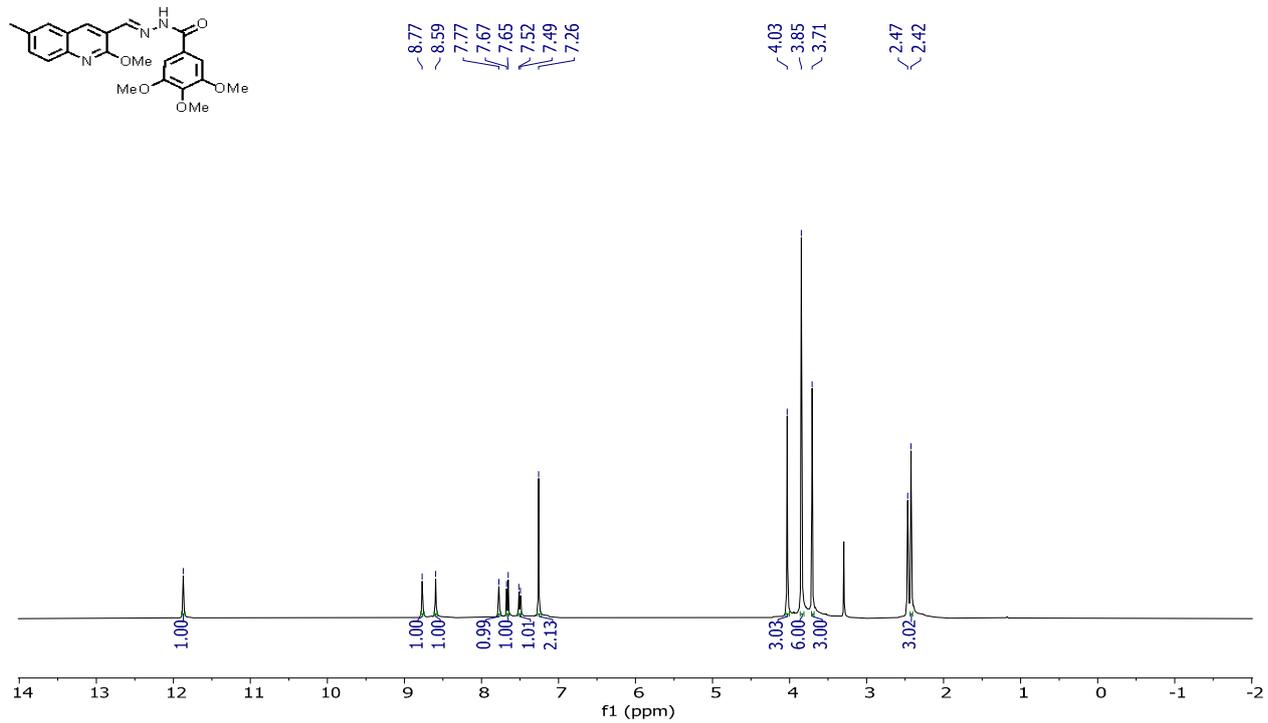


Figure S4; ¹³C NMR for compound 19b

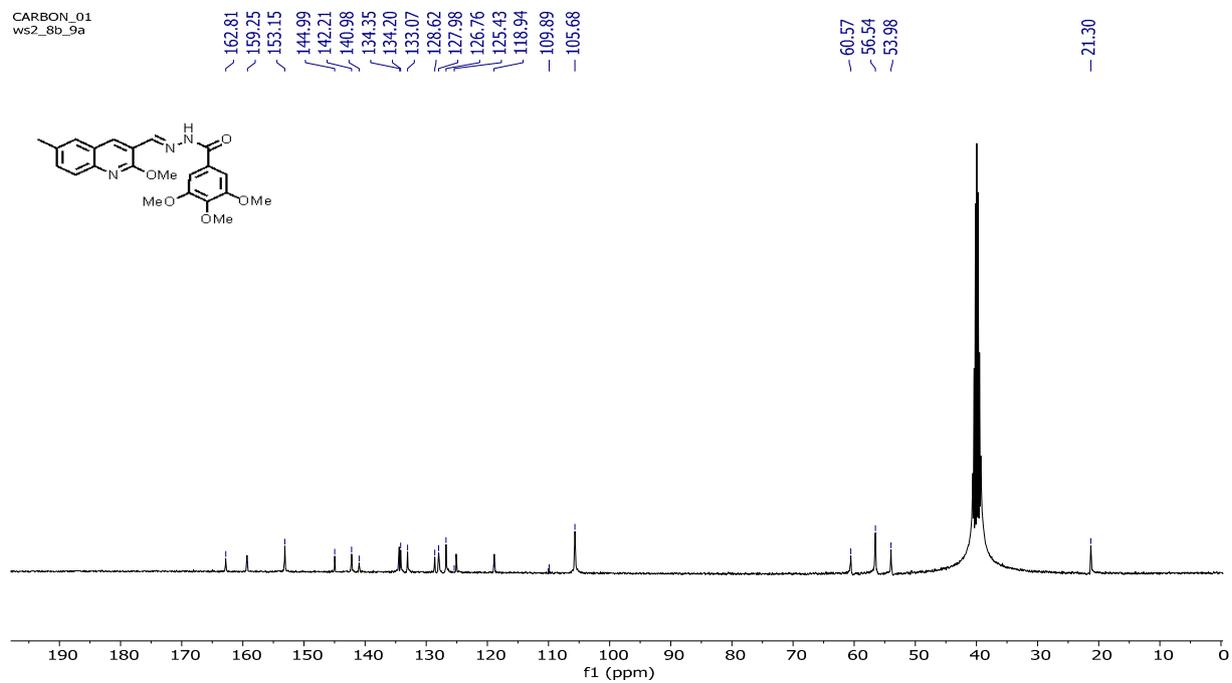


Figure S5; ¹H NMR for compound 19c

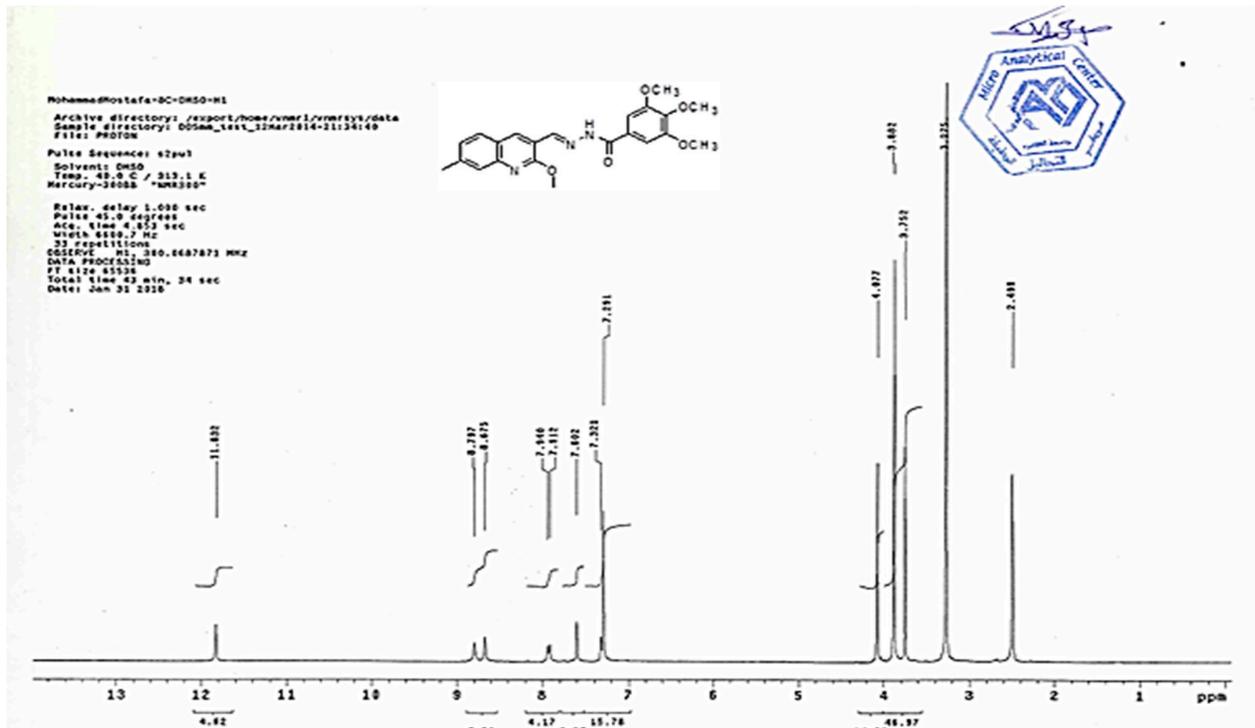


Figure S6; ¹³C NMR for compound 19c

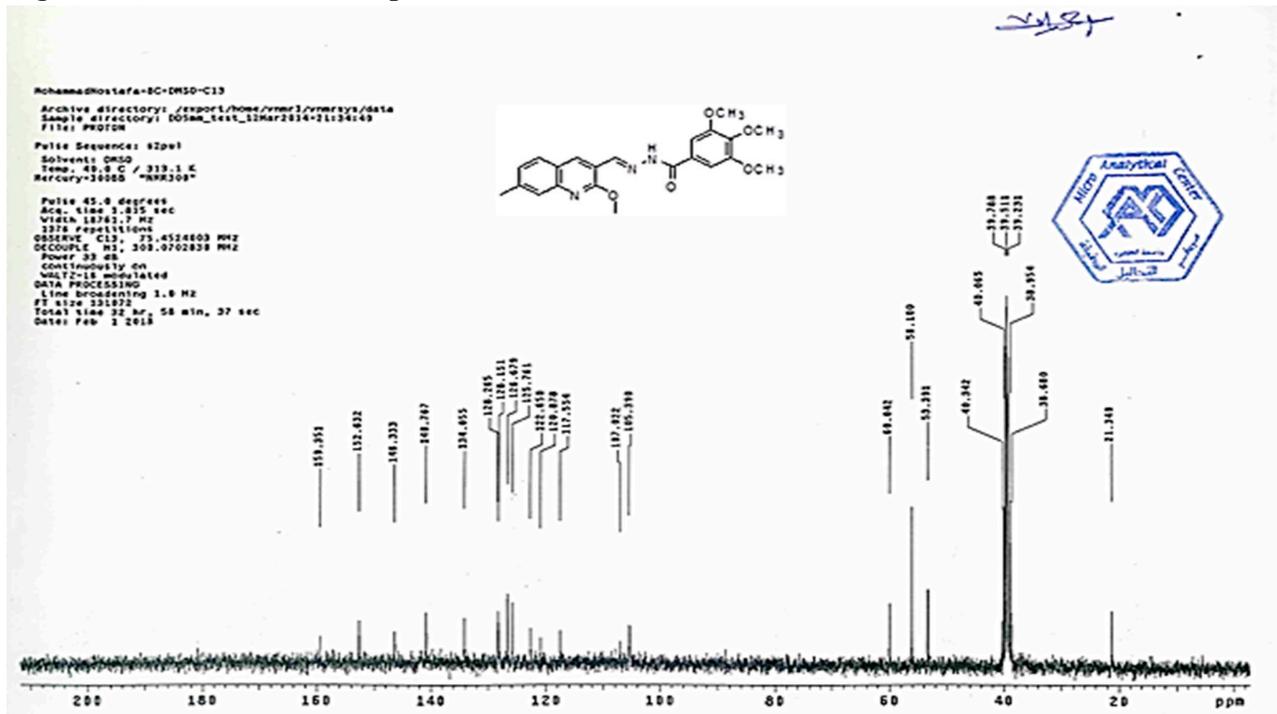


Figure S7; ¹H NMR for compound 19d

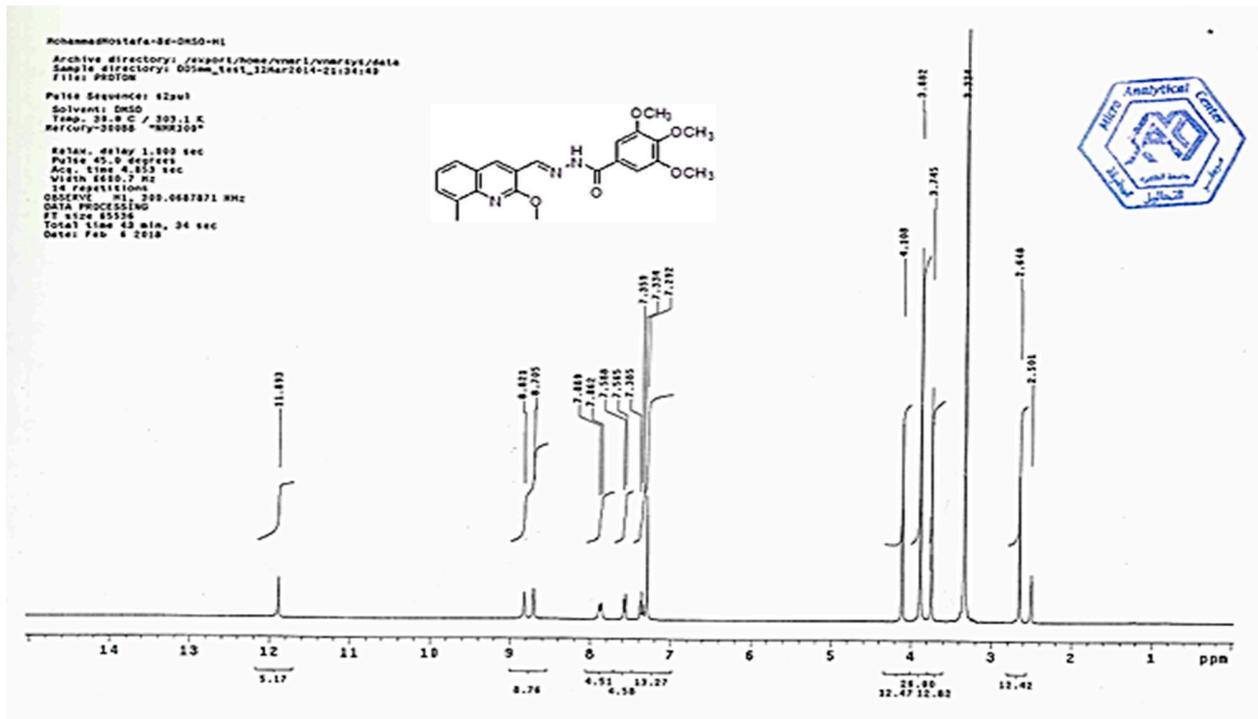


Figure S8; ¹³C NMR for compound 19d

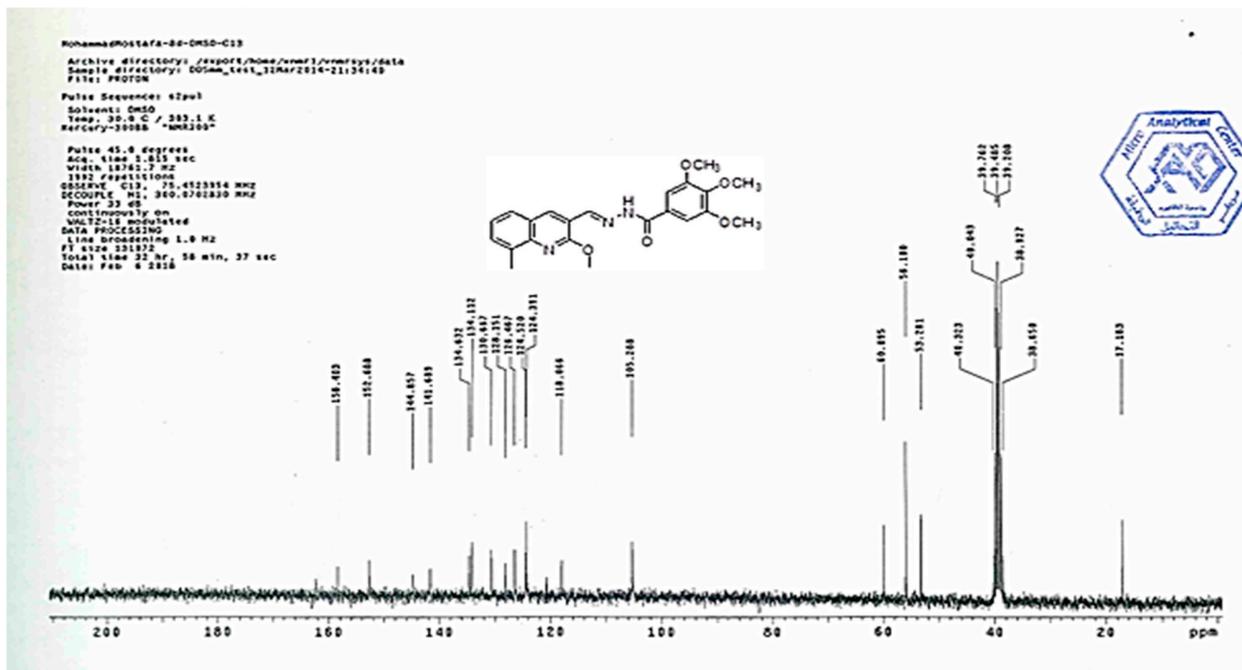


Figure S9; ¹H NMR for compound 19e

Mar27-2017-nmr
MOHAMED-H1
PROTON_BSU DMSO {C:\data} nmr 23

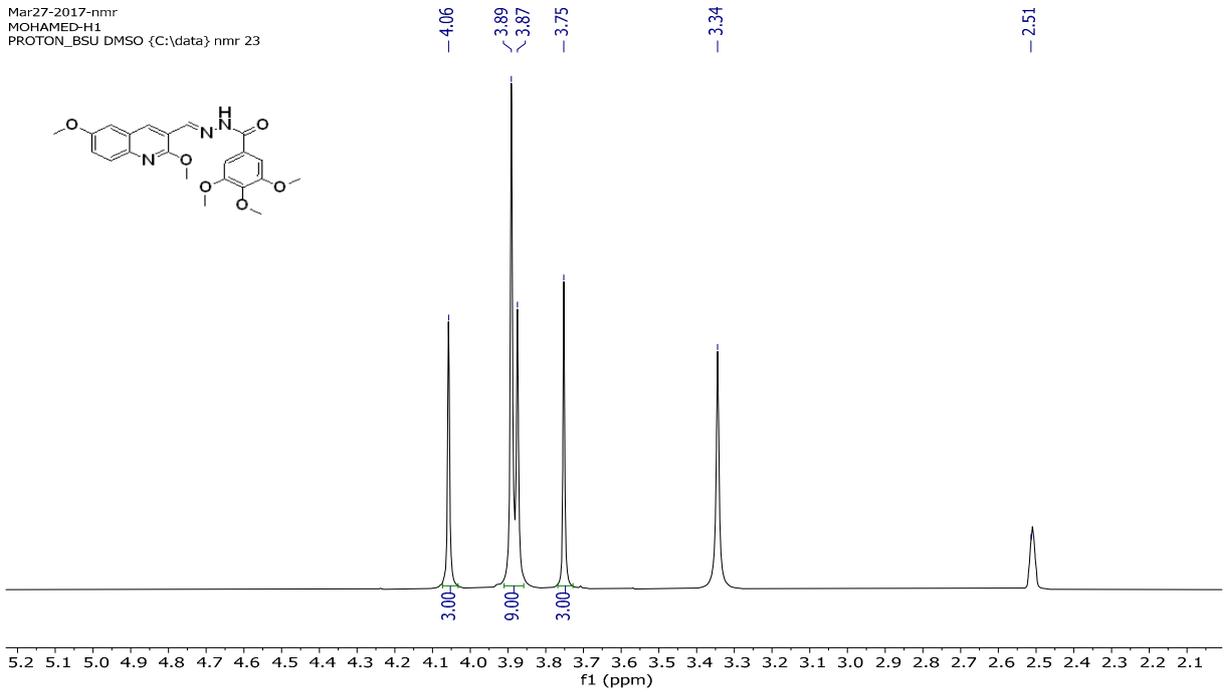


Figure S10; ¹³C NMR for compound 19e

Apr02-2017-nmr
MOHAMED-H1
C13-BSU DMSO {C:\data} nmr

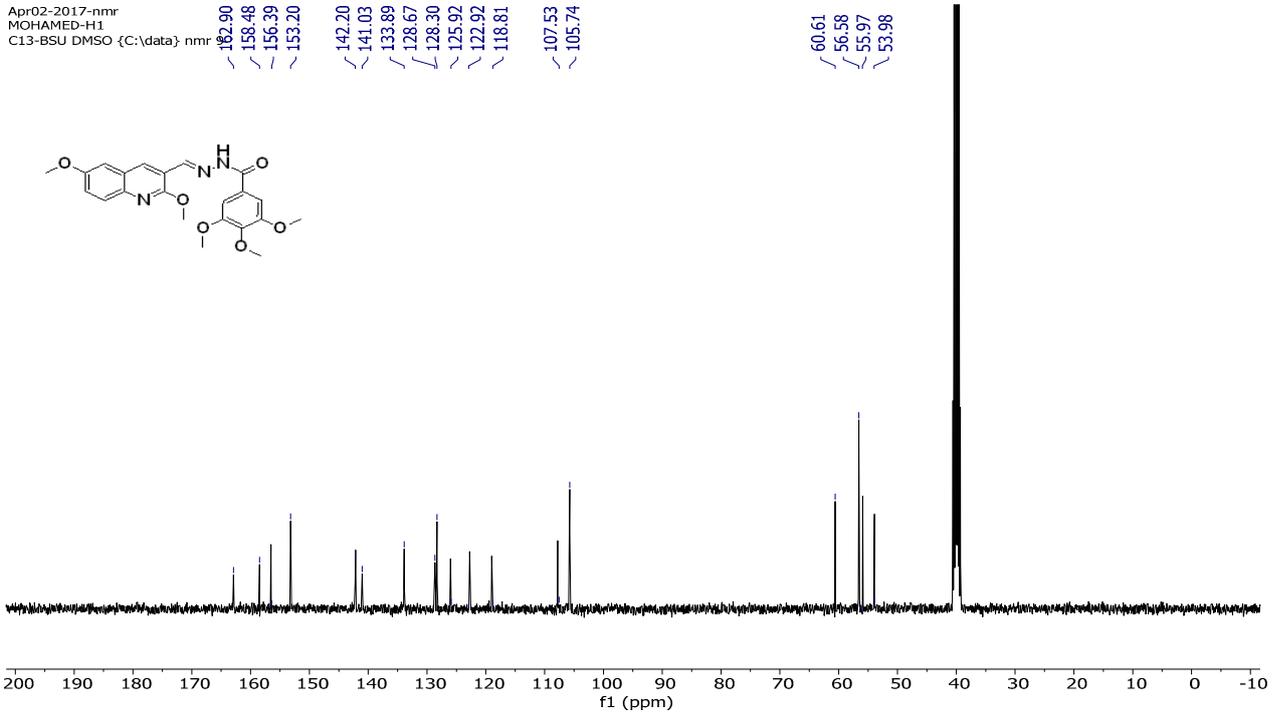


Figure S11; ¹H NMR for compound 19f

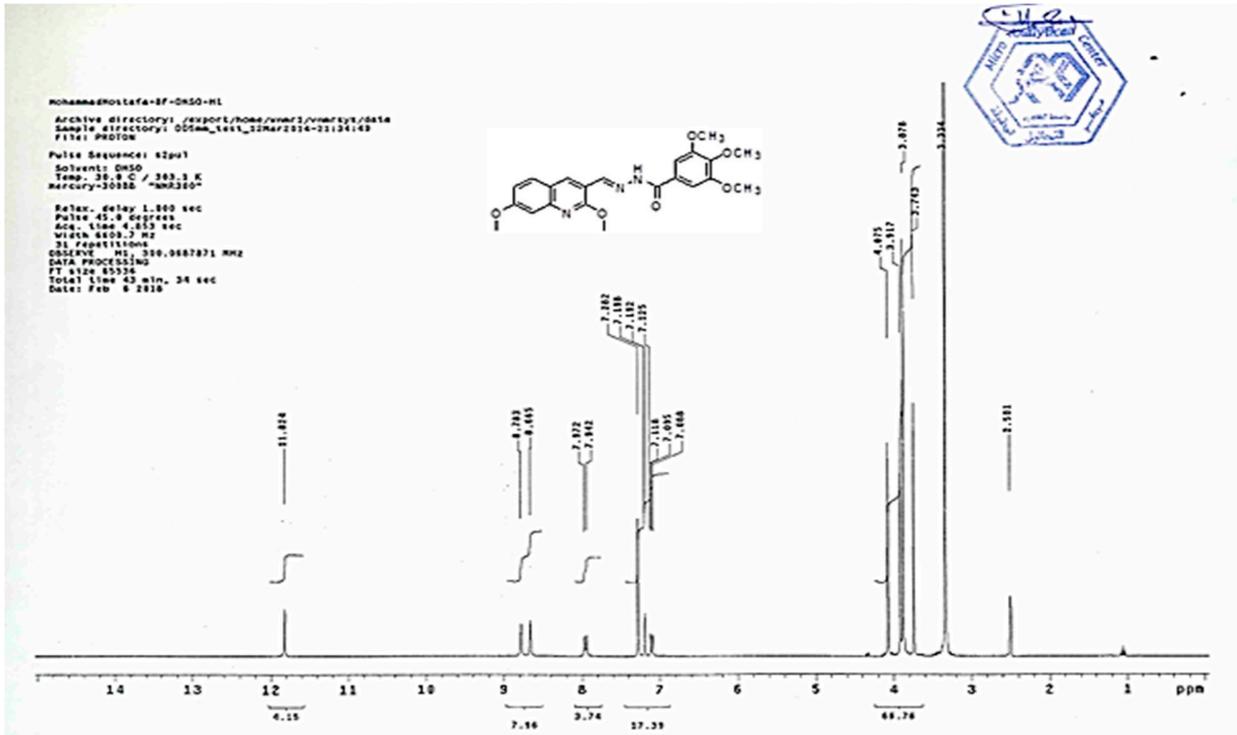


Figure S12; ¹³C NMR for compound 19f

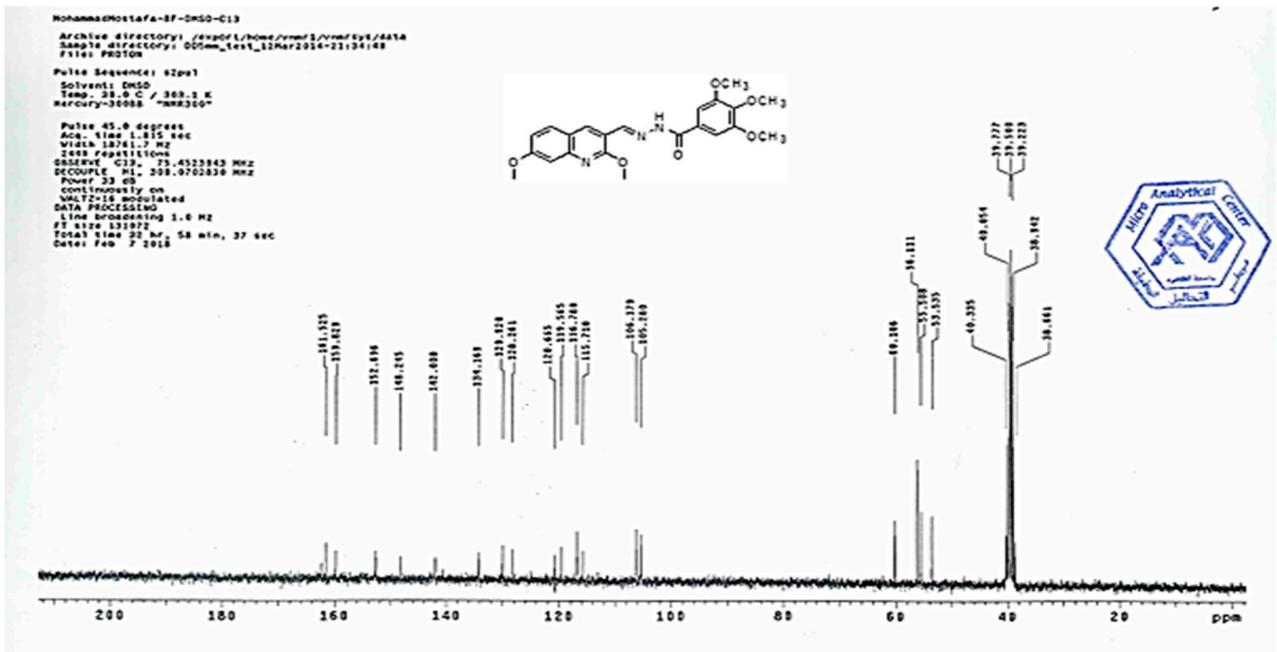


Figure S13; ¹H NMR for compound 19g

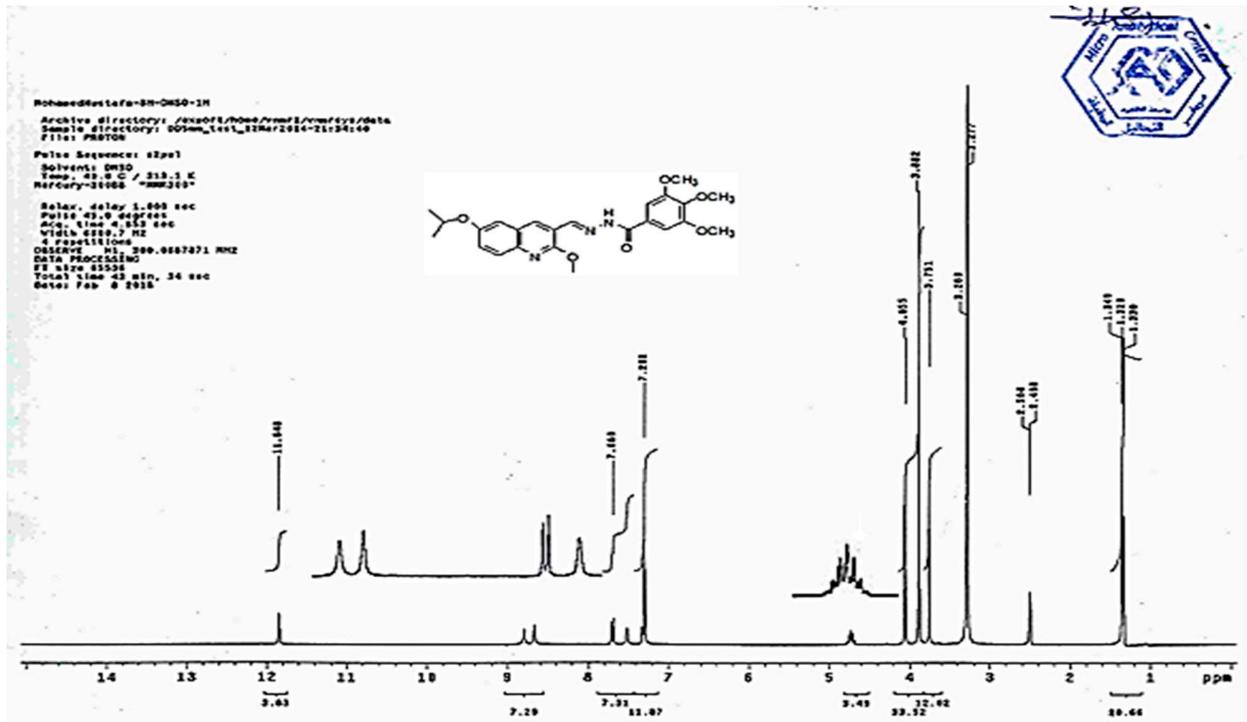


Figure S14; ¹³C NMR for compound 19g

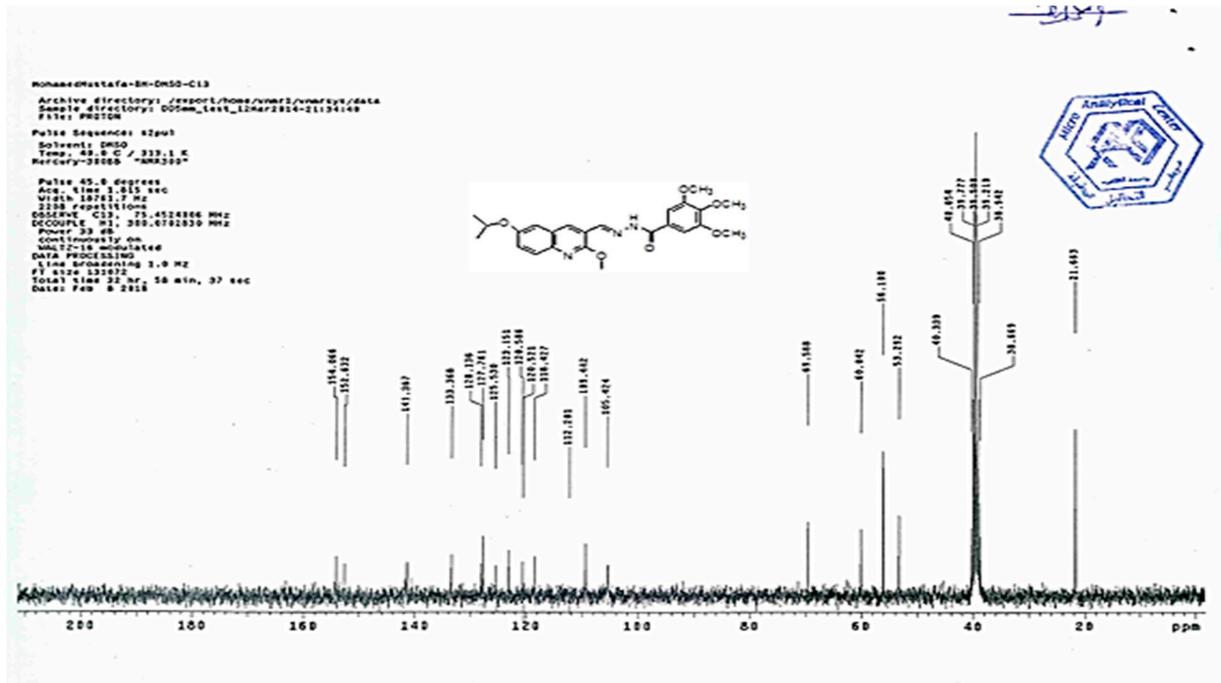


Figure S17; ¹H NMR for compound 19i

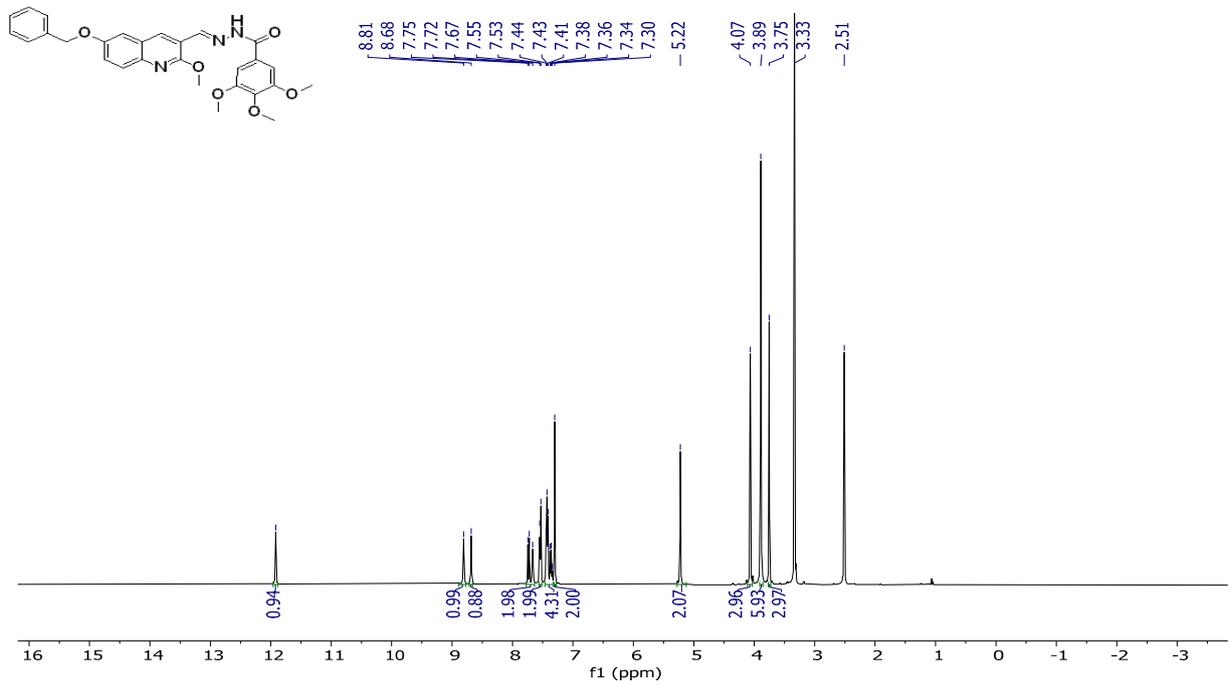


Figure S18; ¹³C NMR for compound 19i

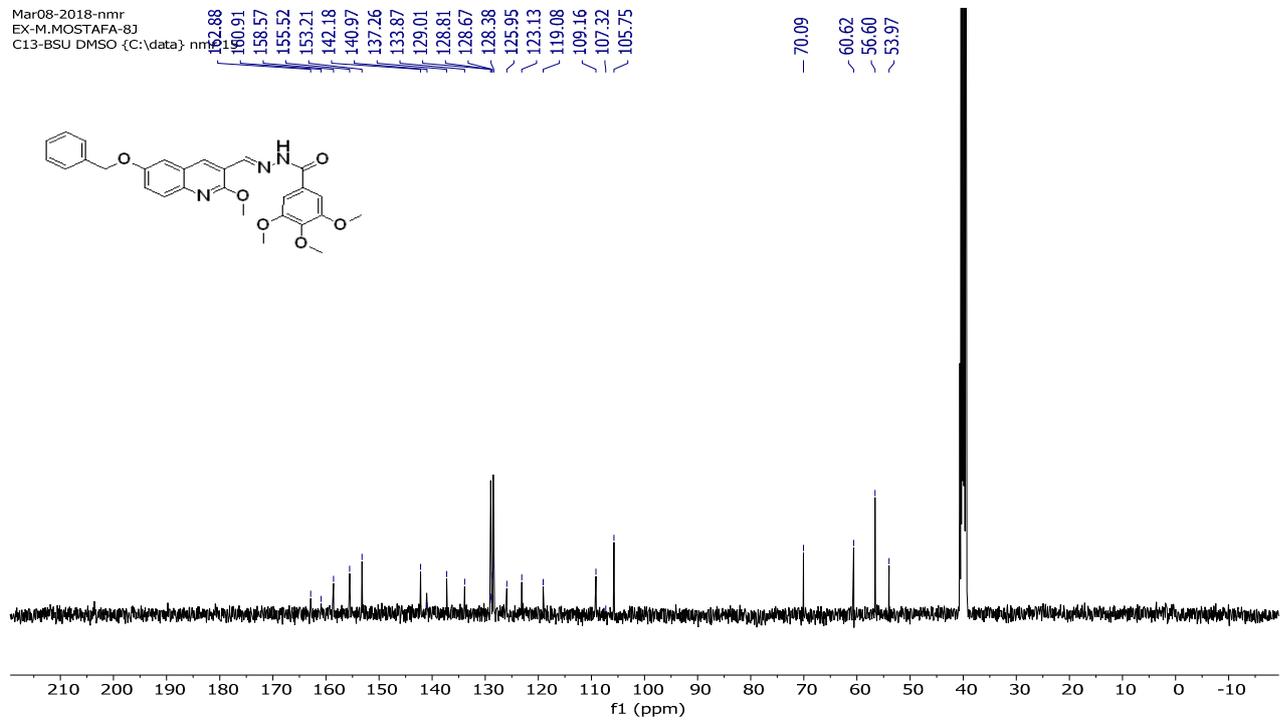


Figure S19; ¹H NMR for compound 19j

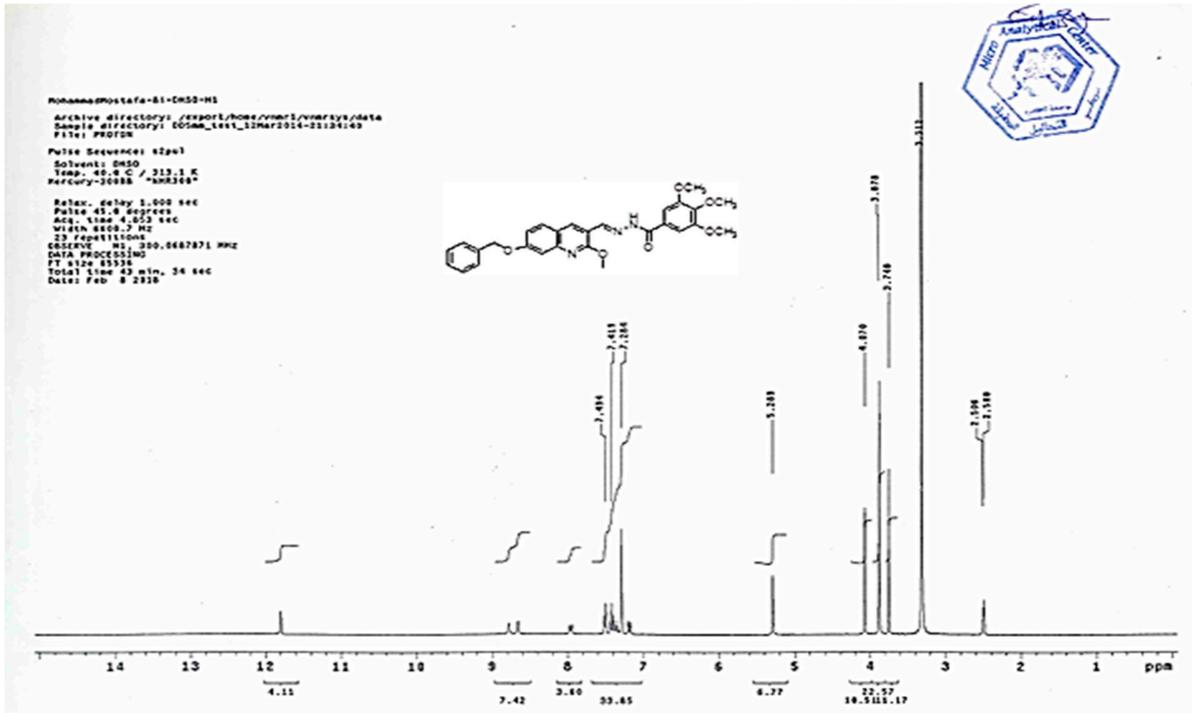


Figure S20; ¹³C NMR for compound 19j

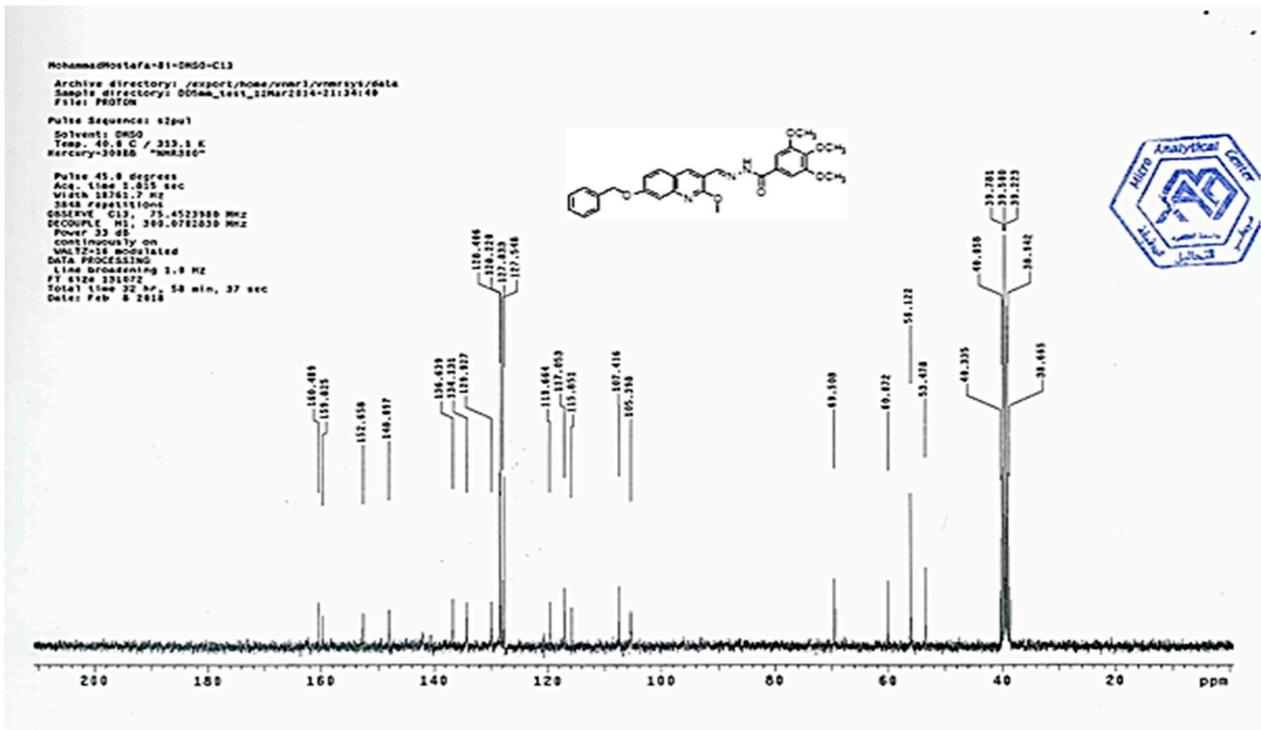


Figure S21; ¹H NMR for compound 20a

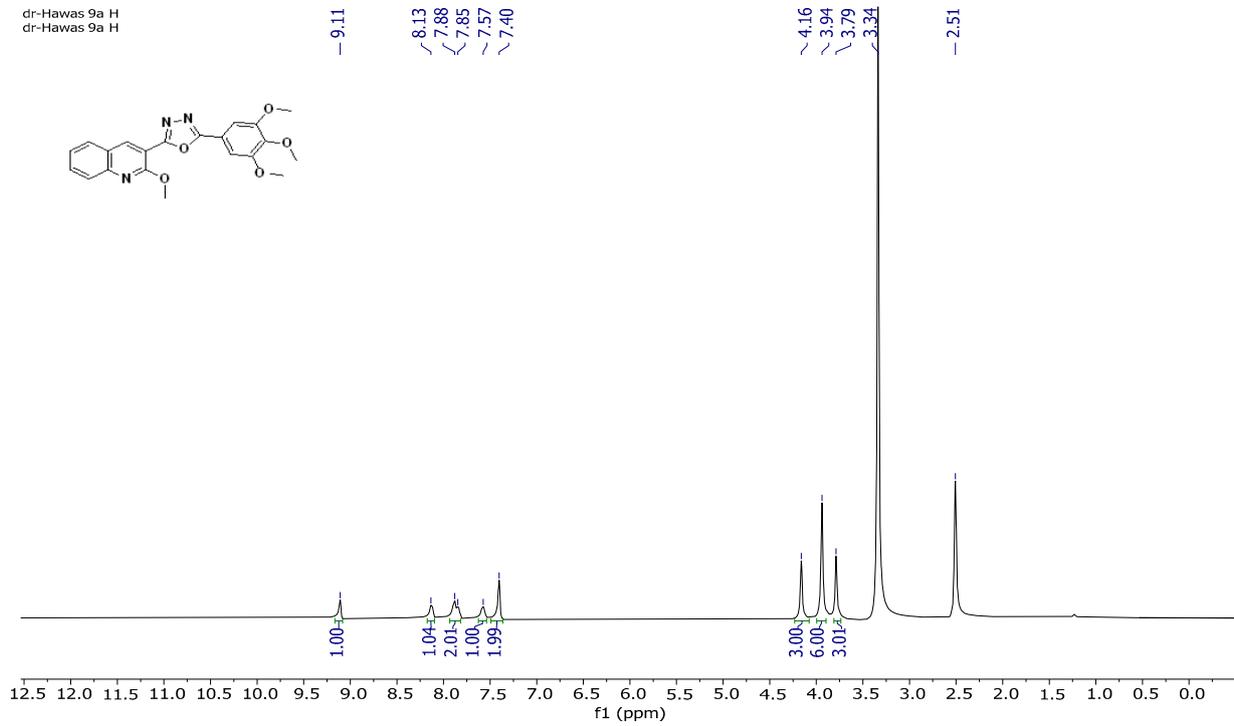


Figure S22; ¹³C NMR for compound 20a

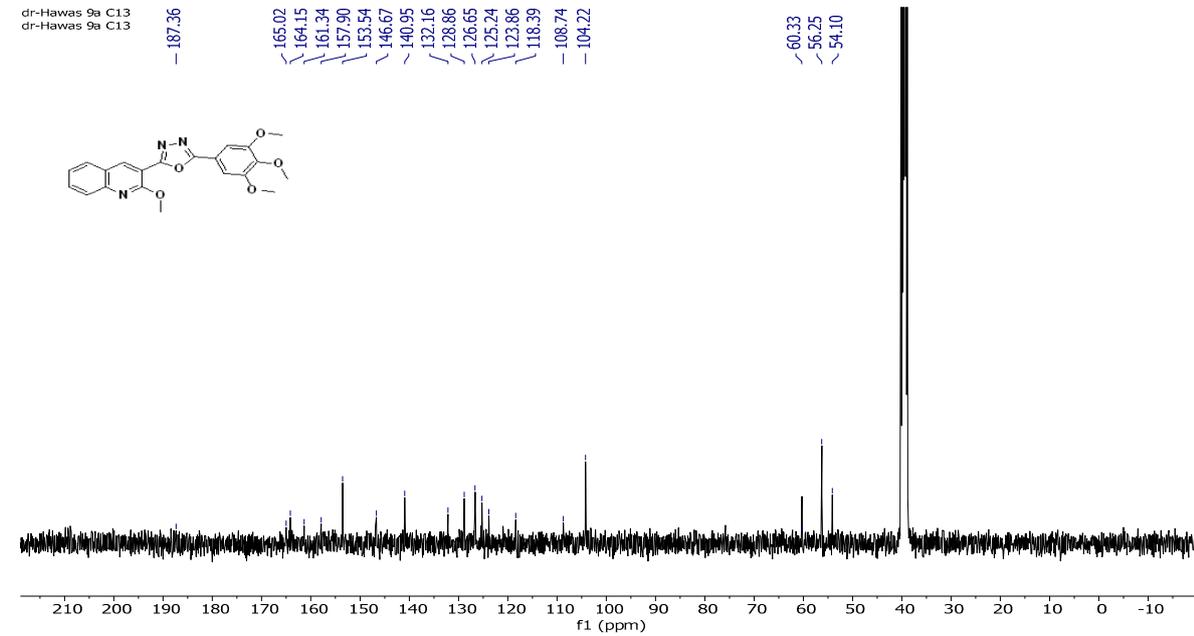


Figure S23; ¹H NMR for compound 20b

Jul02-2018-abeer
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PROTON_BSU DMSO {C:\data\abeer 11

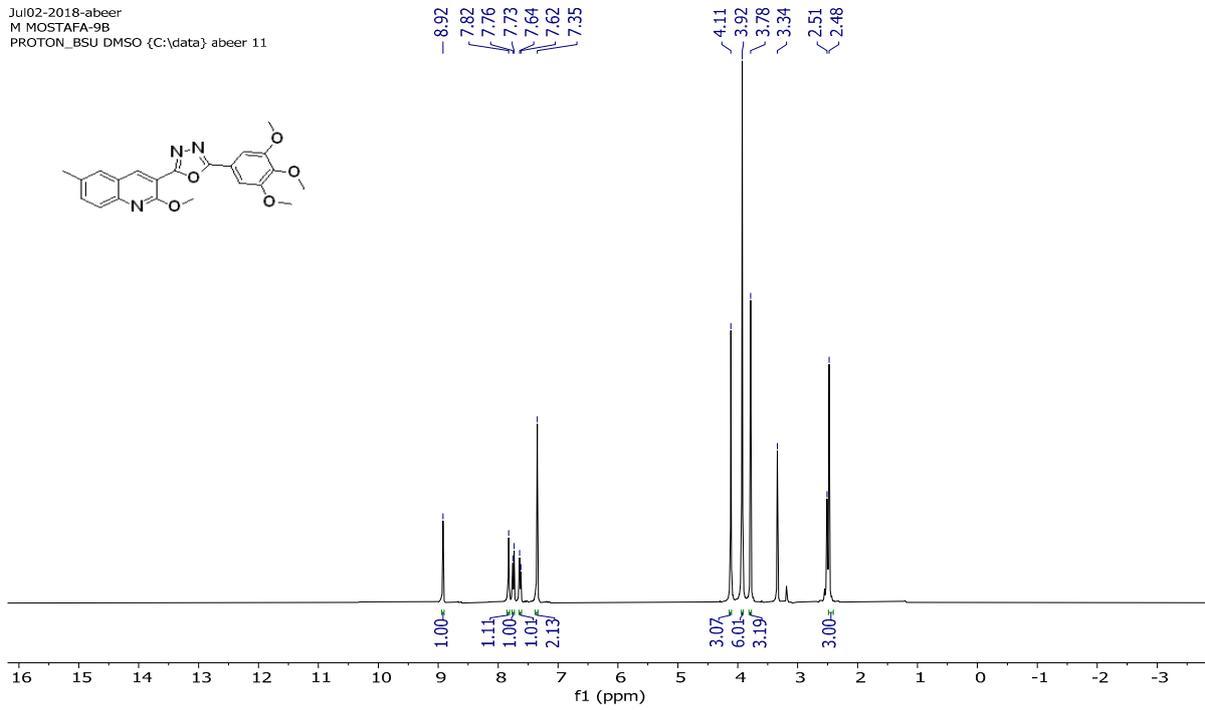


Figure S24; ¹³C NMR for compound 20b

dr-Hawas 9b C13
dr-Hawas 9b C13

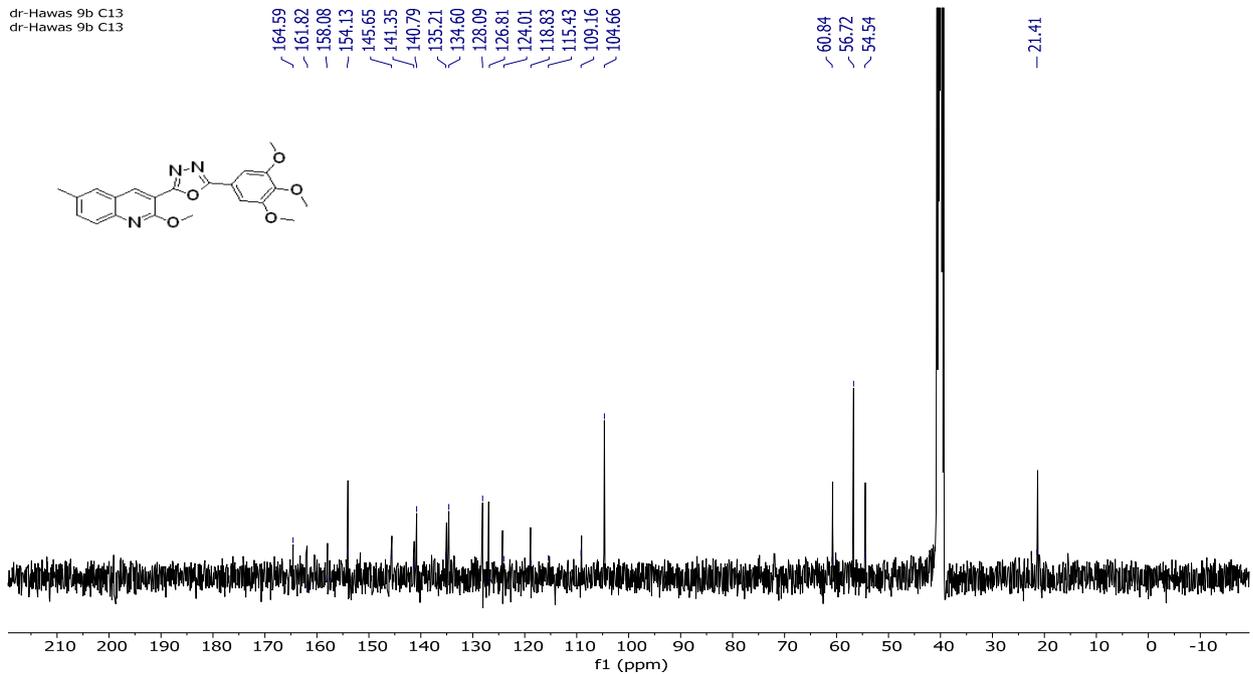


Figure S27; ¹H NMR for compound 20d

Jul02-2018-abeer
M MOSTAFA-9D
PROTON_BS DMSO {C:\data} abeer 10

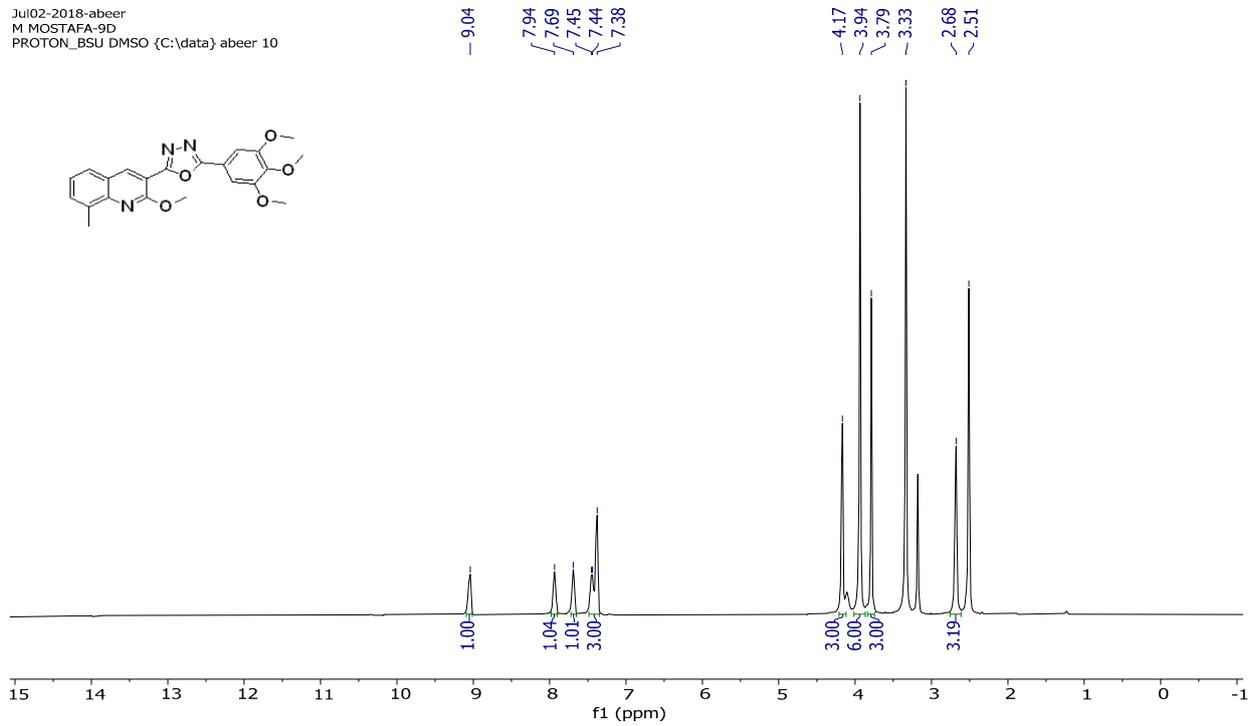


Figure S28; ¹³C NMR for compound 20d

dr-Hawas 9d C13
dr-Hawas 9d C13

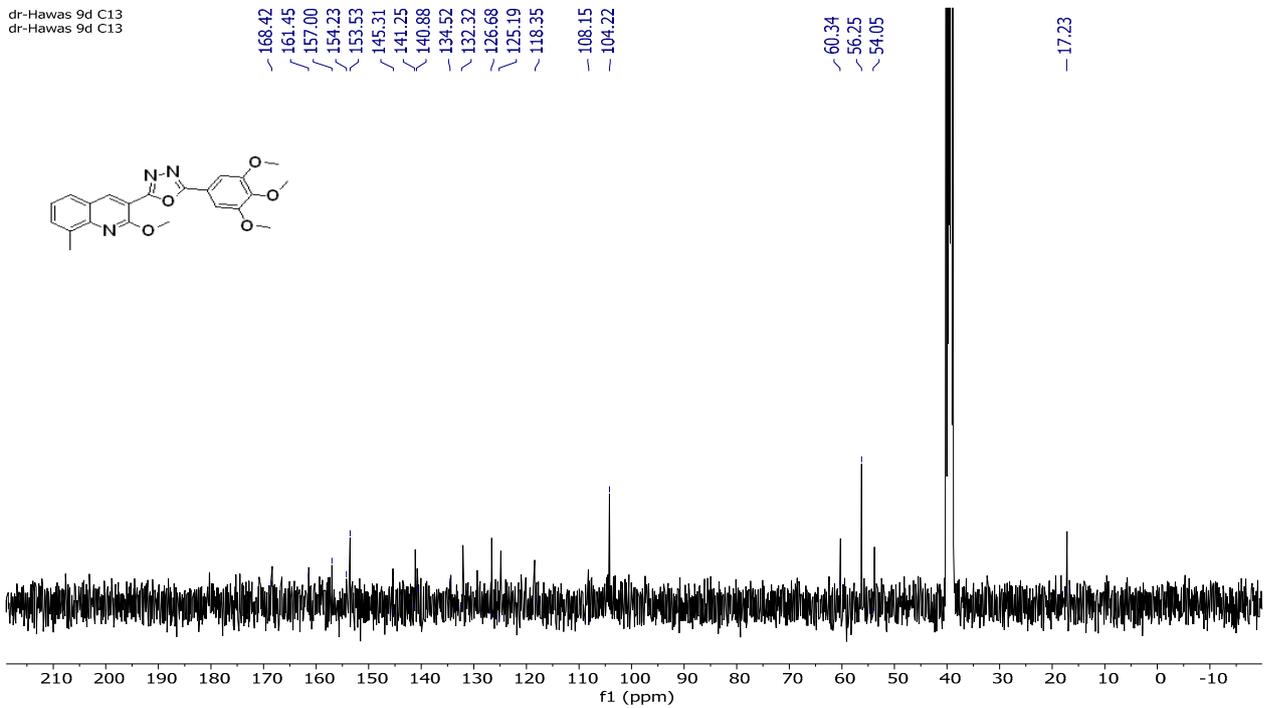


Figure S29; ¹H NMR for compound 20e

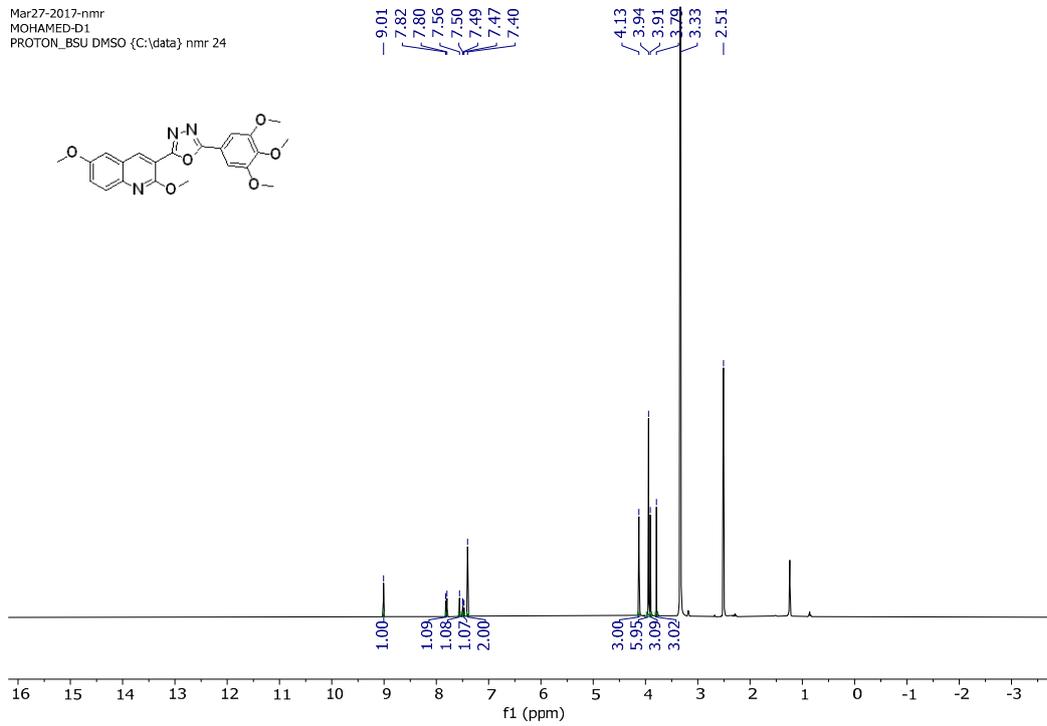


Figure S30; ¹³C NMR for compound 20e

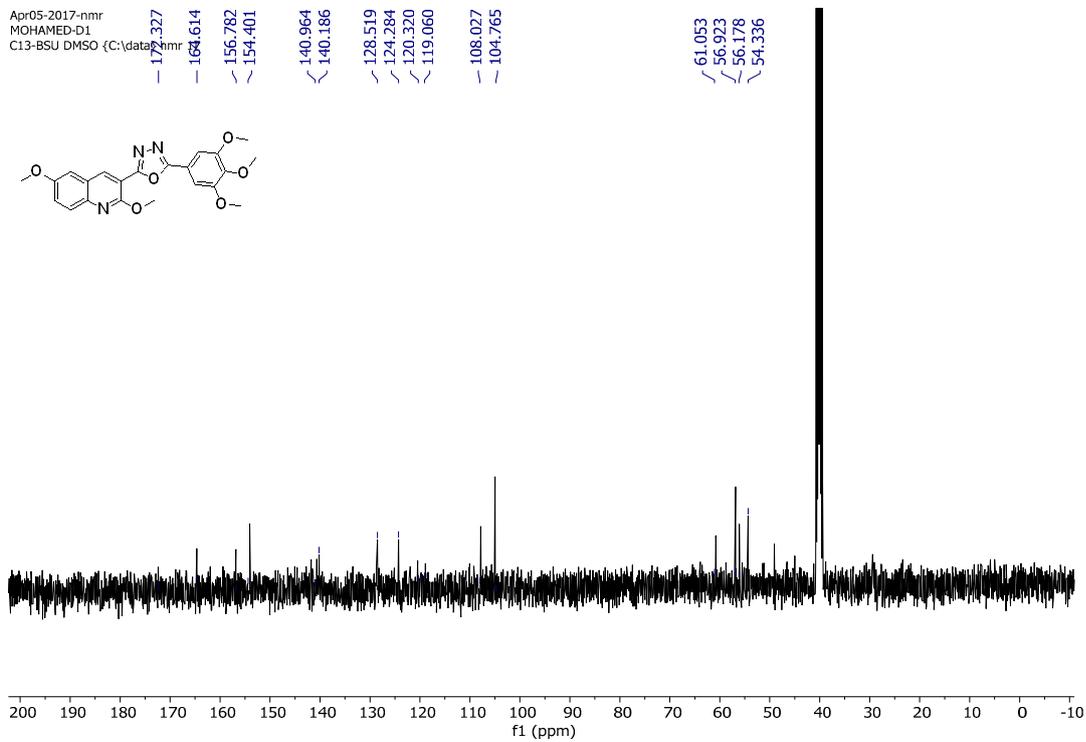


Figure S31; ¹H NMR for compound 20f

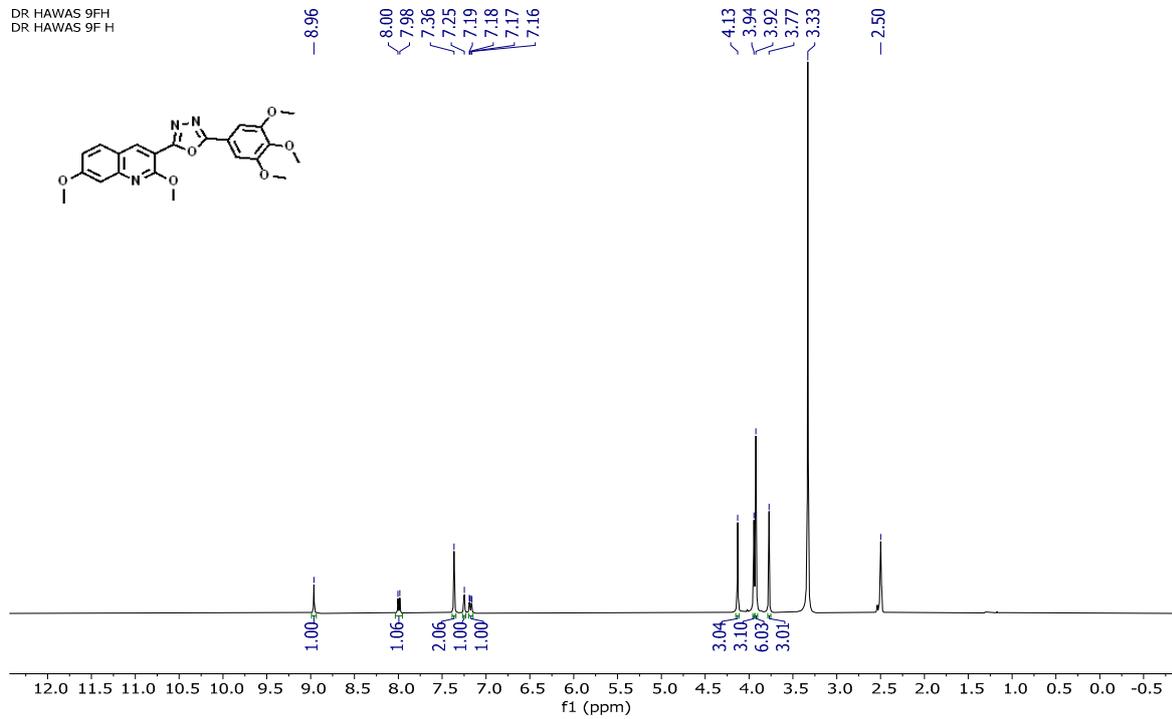


Figure S32; ¹³C NMR for compound 20f

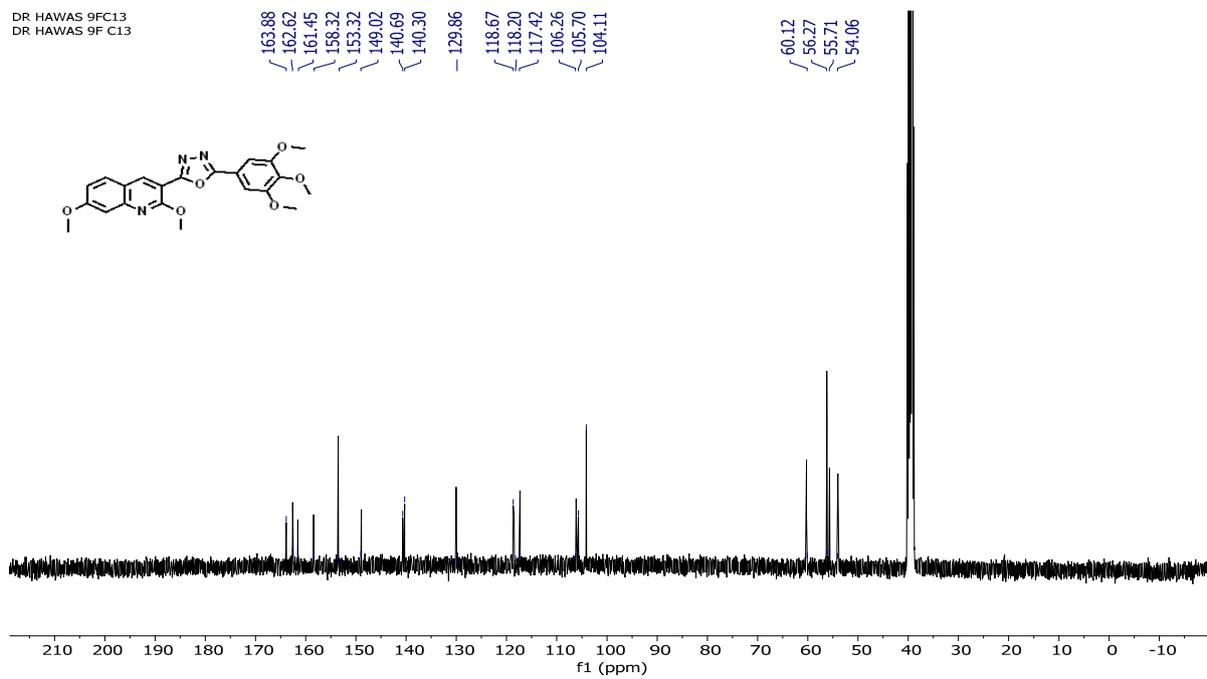


Figure S33; ¹H NMR for compound 20g

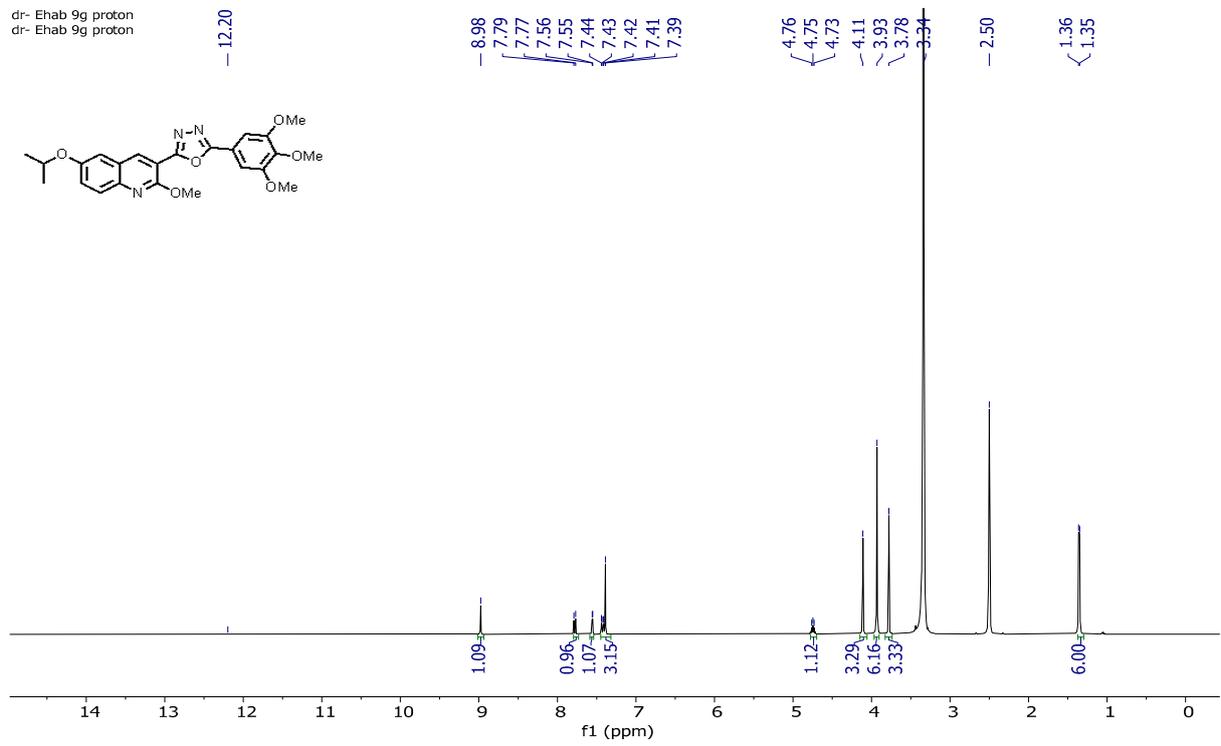


Figure S34; ¹³C NMR for compound 20g

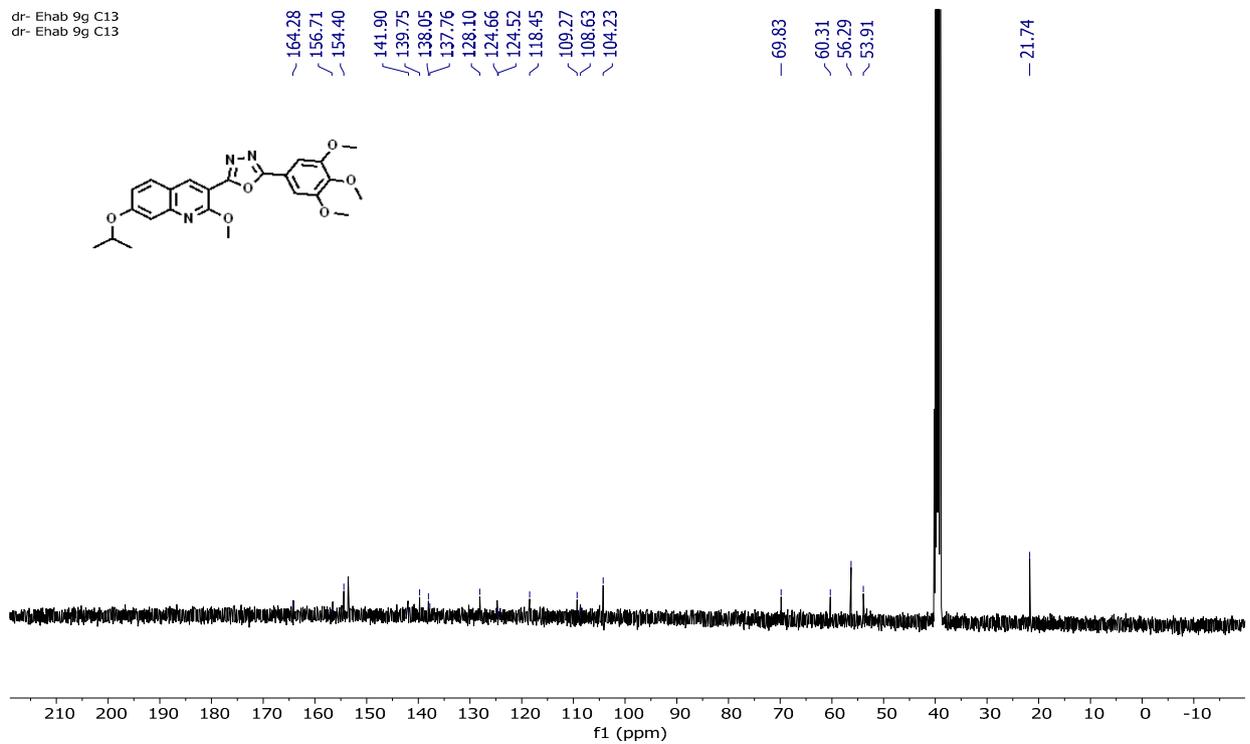


Figure S35; ¹H NMR for compound 20h

Jul02-2018-abeer
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PROTON_BSU DMSO {C:\data} abeer 12

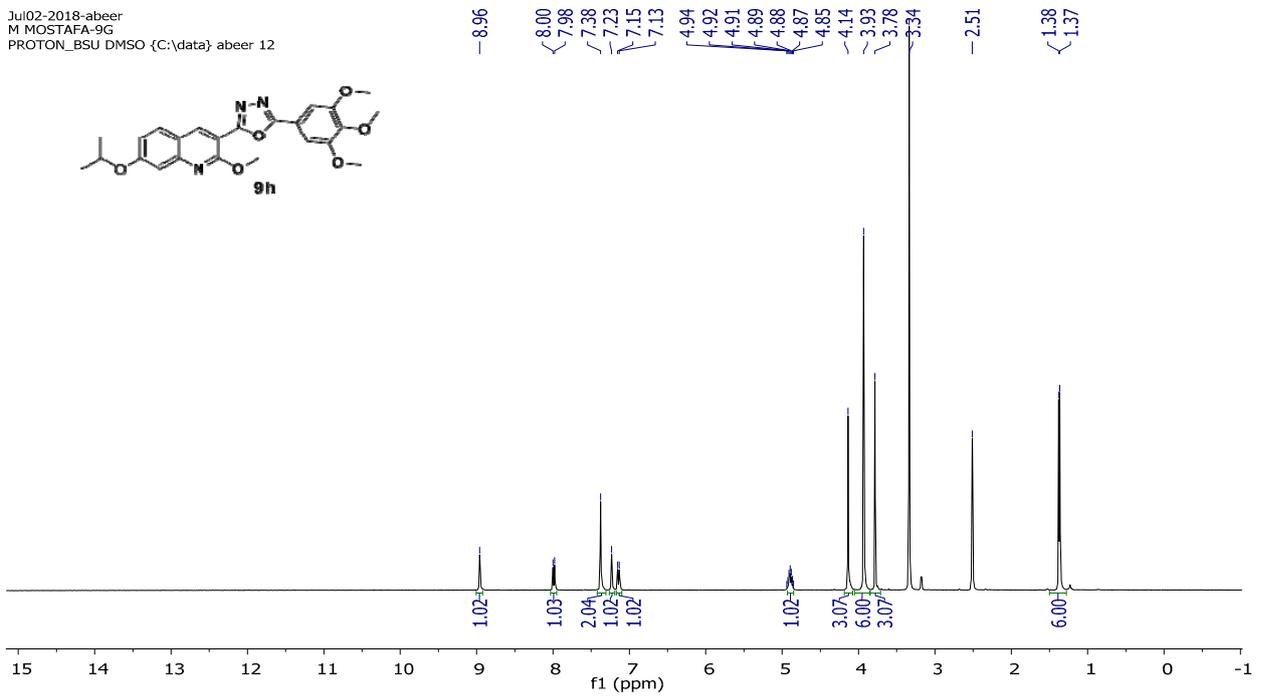


Figure S36; ¹³C NMR for compound 20h

dr-Hwas 9h C13
dr-Hawas 9h C13

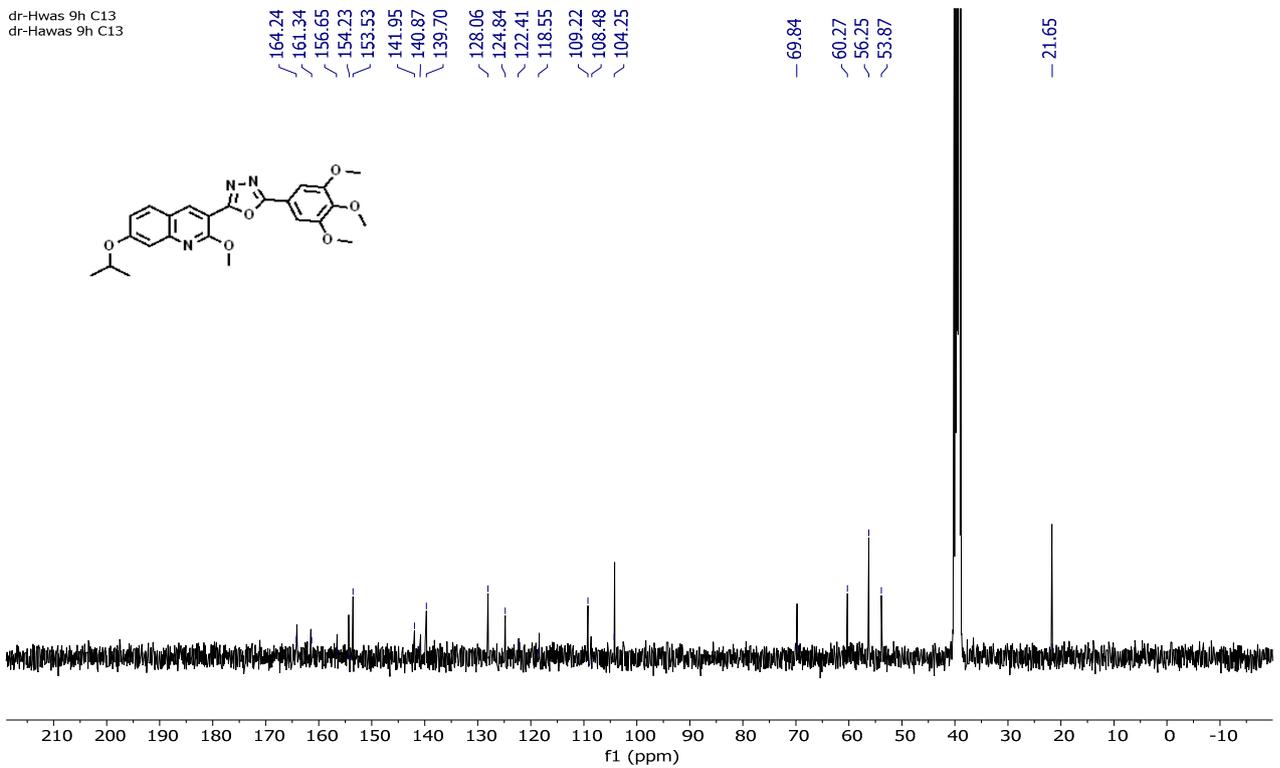


Figure S37; ¹H NMR for compound 20i

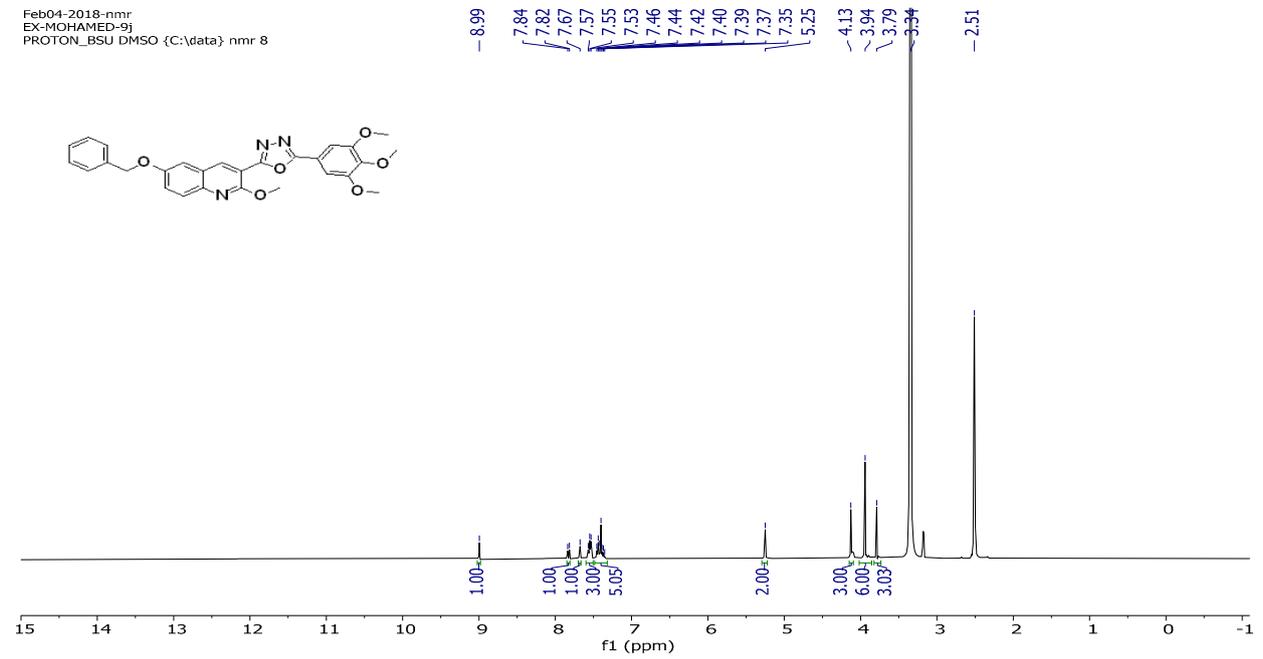


Figure S38; ¹³C NMR for compound 20i

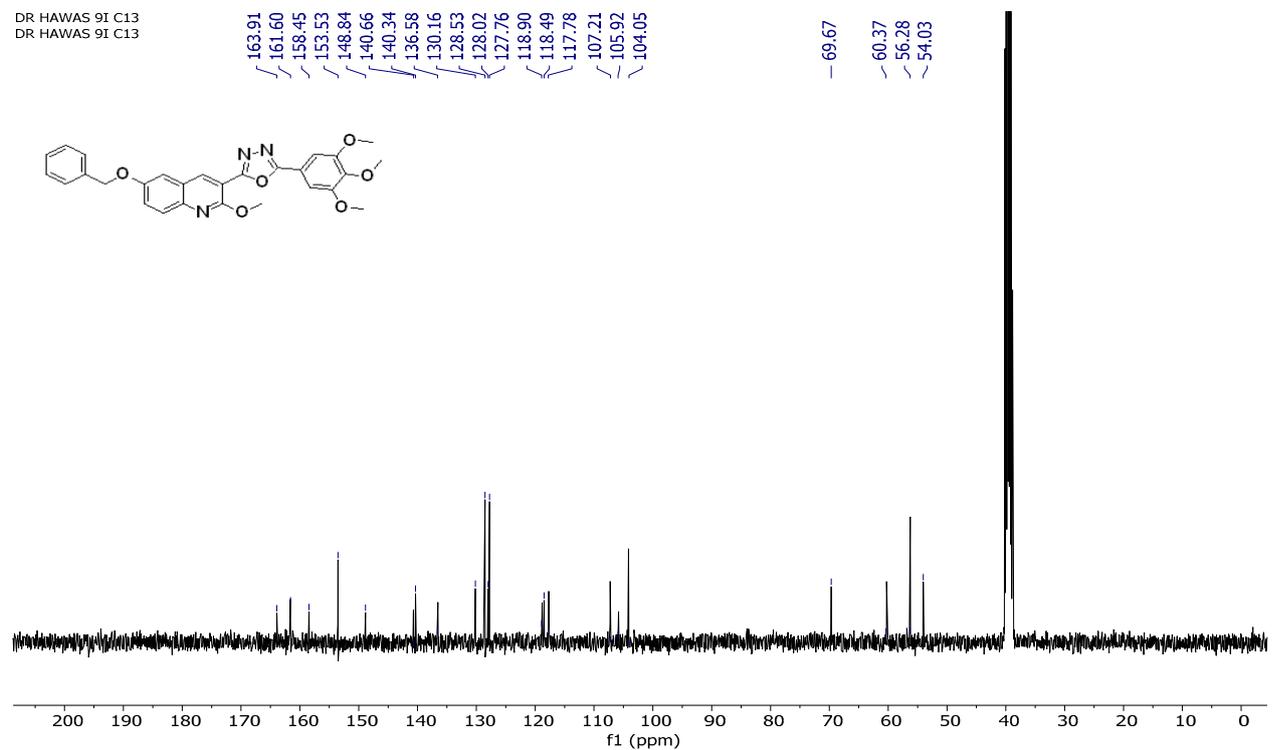


Figure S39; ¹H NMR for compound 20j

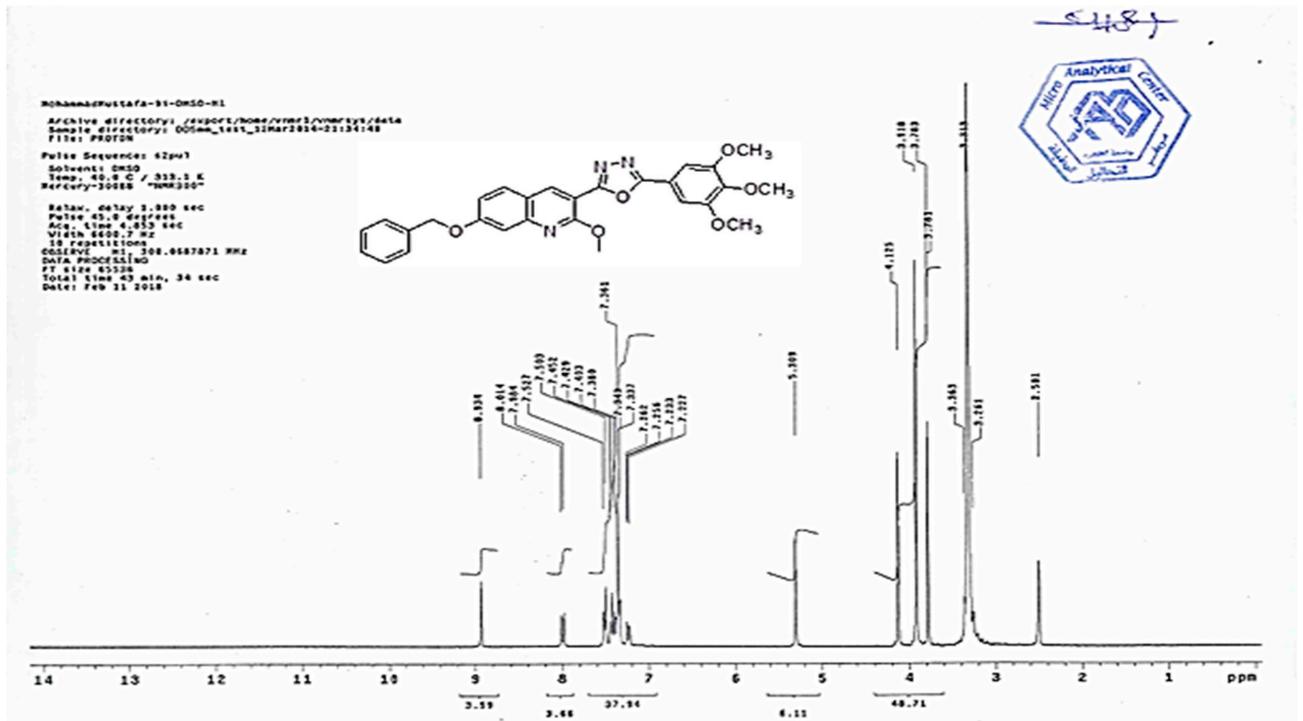
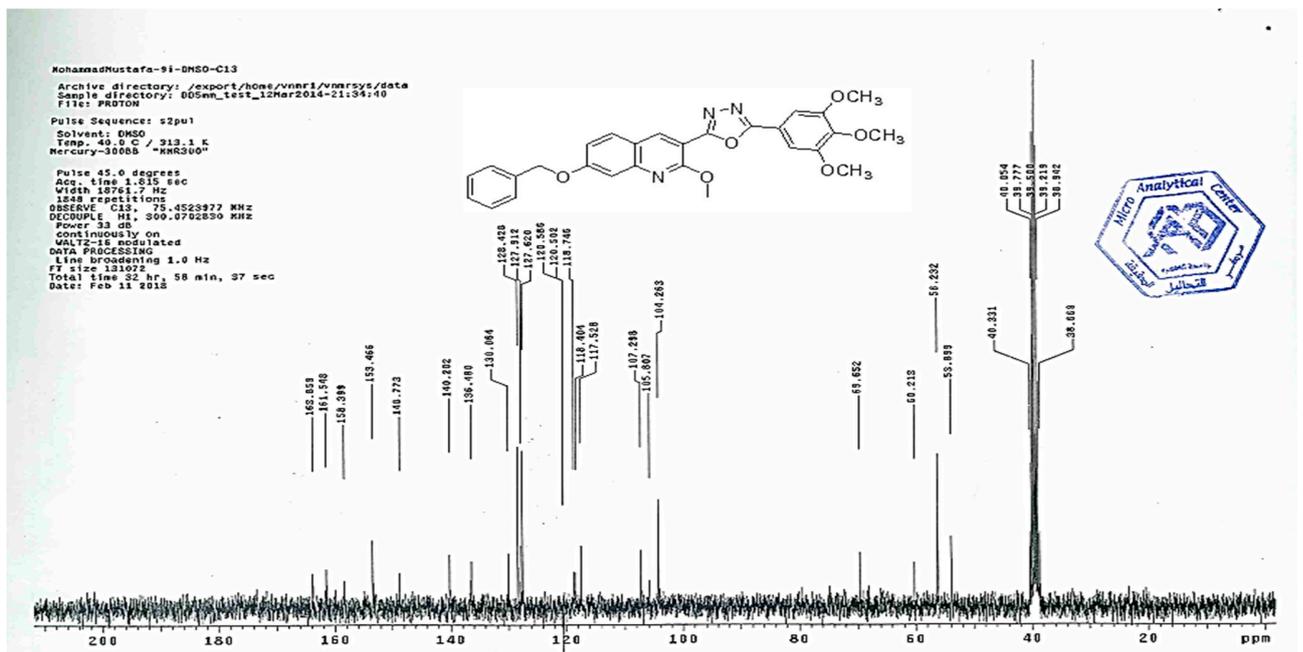


Figure S40; ¹³C NMR for compound 20j



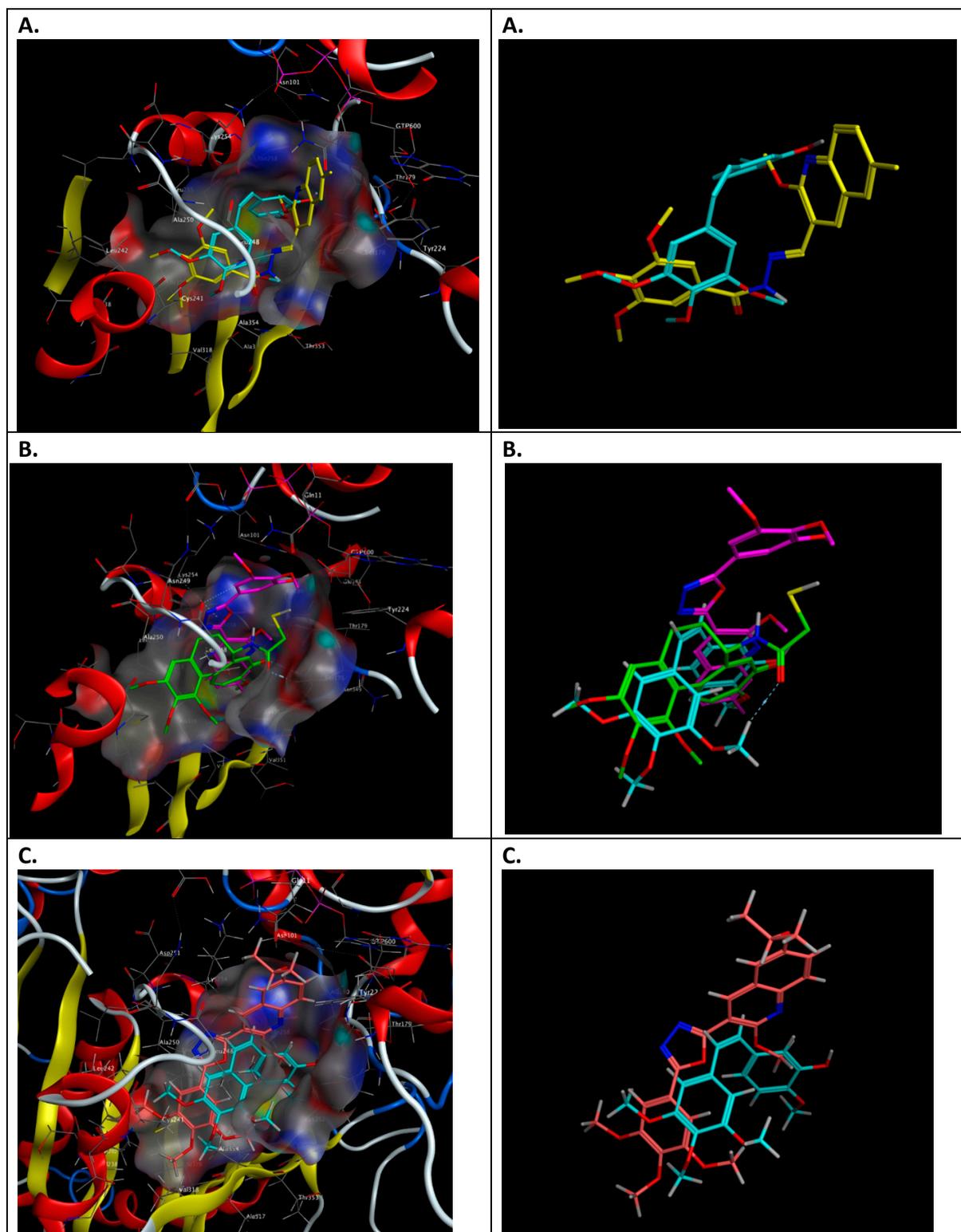


Figure S41. **A.** Quinoline **19b** (yellow) and CA-4 (cyan) docked at the colchicine-binding site of tubulin in co-crystal 1SAO. **B.** Quinoline **20c** (pink) and DAMA-colchicine (green) docked at the colchicine-binding site of tubulin in co-crystal 1SAO. **C.** Quinoline **9=20g** (red) and CA-4 (cyan) docked at the colchicine-binding site of tubulin in co-crystal 1SAO. Protein residues removed on right for clarity. (red = oxygen, grey = hydrogen).

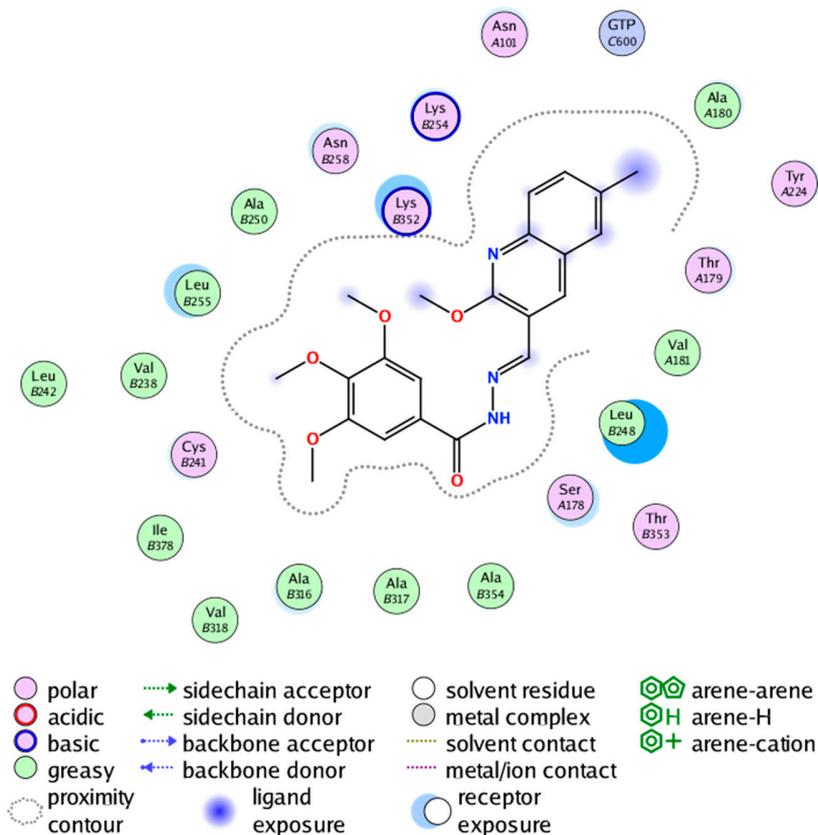


Figure S42. 2D Ligand Interaction Schematic for **19b** as generated by MOE

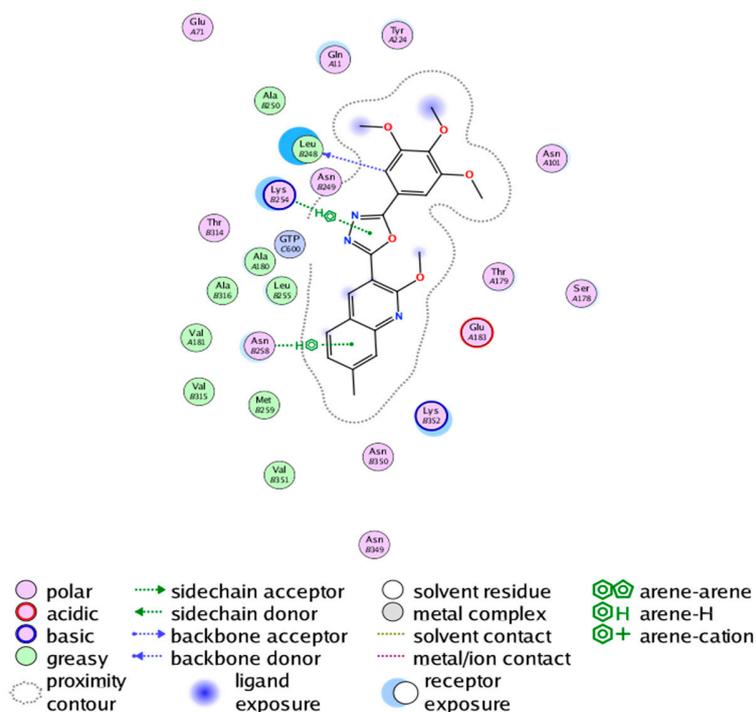


Figure S43. 2D Ligand Interaction Schematic for **20c** as generated by MOE

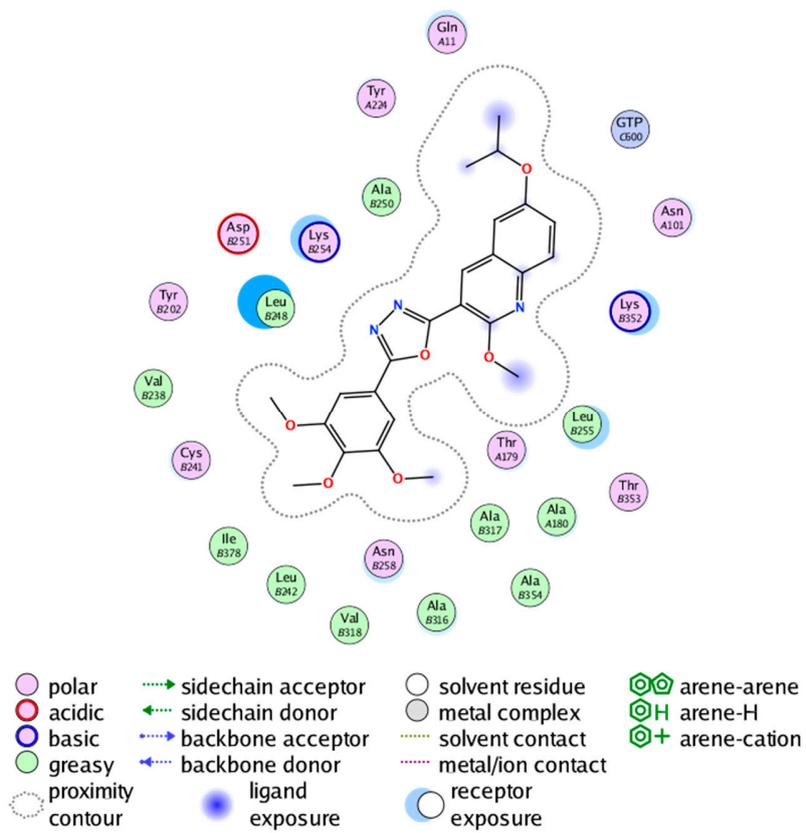


Figure S44. 2D Ligand Interaction Schematic for **20g** as generated by MOE